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Entropy Production in Quantum Brownian Motion

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Abstract

We investigate how to coherently define entropy production for a process of transient relaxation in the Quantum Brownian Motion model for the harmonic potential. We compare a form, called "Poised" (P), which after non-Markovian transients corresponds to a definition of heat as the change in the system Hamiltonian of mean force, with a recent proposal by Esposito *et al* (ELB) based on a definition of heat as the energy change in the bath. Both expressions yield a positive-defined entropy production and coincide for vanishing coupling strength, but their difference is proved to be always positive (after non-Markovian transients disappear) and to grow as the coupling strength increases. In the classical over-damped limit the "Poised" entropy production converges to the entropy production used in stochastic thermodynamics. We also investigate the effects of the system size, and of the ensuing Poincaré recurrences, and how the classical limit is approached. We close by discussing the strong- coupling limit, in which the ideal canonical equilibrium of the bath is violated.

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Contents

Introduction

The theory of stochastic thermodynamics provides a consistent description of nonequilibrium thermodynamics for classical systems weakly coupled to their environments and described by Markovian dynamics [Esposito, 2012, Seifert, 2008]. In recent years fundamental characteristics of classical thermodynamics have been put under scrutiny in the quantum realm where a proper formulation of nonequilibrium thermodynamics seems a much harder task. In particular when considering low temperatures and non-vanishing couplings various difficulties arise, some of which are already present at equilibrium. An ubiquitous exactly solvable model to address these questions is the Quantum Brownian Motion (QBM) model [Ullersma, 1966, Haake and Reibold, 1985, Caldeira and Leggett, 1983]. It consists of a system with Hamiltonian H_S (often an harmonic oscillator) bi-linearly coupled via a term denoted H_I to a bath of harmonic oscillators with Hamiltonian H_B. The total Hamiltonian is thus of the form $H = H_S + H_B + H_I$. In this model, when the total system is initially in canonical equilibrium $\rho^{eq} = e^{-\beta H}/Z$, the Clausius formulation of the second law seems to be violated for a quasi-static change of the mass or of the frequency of the central oscillator [Allahverdyan and Nieuwenhuizen, 2000, Hörhammer and Büttner, 2008]. In this case, the heat flow is defined as the change in the averaged central system Hamiltonian due to the bath and is found to be larger than the temperature times the change in the system entropy, defined as the von Neumann entropy of the central system. To remain consistent with these definitions, work and free energy are also defined in terms of the system Hamiltonian and as a result the Thompson formulation of the second law is also violated [Ford and O'Connell, 2006, Nieuwenhuizen and Allahverdyan, 2002]. More work can be extracted from the system than the change in its free energy. One also intriguingly finds that the behavior of the heat capacity of the system is different when it is derived from the energy of the central system at equilibrium or from a partition function approach [Hänggi et al., 2008, Hänggi and Ludwig Ingold, 2006]. In this latter case the heat capacity might even become negative at low temperature. Also, the von Neumann entropy of the central oscillator does not vanish at zero temperature while the equilibrium entropy of the total system (which coincides with the von Neumann entropy of the total system)

does. These phenomena can be ascribed to quantum correlations between the central system and the bath [Hilt and Lutz, 2009]. Various attempts have been made in order to overcome these difficulties. Some of them incorporate in Thompson's formulation of the second law the work contribution required to initially couple the system to the bath at zero [Ford and O'Connell, 2006] or arbitrary temperatures [Hilt et al., 2011, Kim and Mahler, 2007]. Others introduce different notions of effective temperature [Nieuwenhuizen and Allahverdyan, 2002, Kim and Mahler, 2010]. Ultimately, many of the difficulties are related to the fact that the equilibrium density matrix of the central oscillator is not the familiar canonical distribution $\rho_{\mathrm{S}}^{\mathrm{eq}} = \mathrm{e}^{-\beta H_{\mathrm{S}}}/Z_{\mathrm{S}}$ defined in terms of the central system Hamiltonian as is often the case in weak-coupling theories.

In this thesis, we want to investigate the slightly different problem of transient relaxation to equilibrium in the QBM model. This means that we initially place the central oscillator in a nonequilibrium state and put it in contact with its bath at equilibrium. Due to the interaction, the two parts of the system will exchange energy and if the bath is sufficiently large, the central oscillator will asymptotically reach an equilibrium state. For such a process we would like to identify a meaningful notion of entropy production. In stochastic thermodynamics the nonequilibrium version of the second law states that for such a relaxation process the entropy production is equal to the change in system entropy (which is identified with the Shannon entropy of the system) minus the heat exchanged with the bath divided by the bath temperature. Furthermore the entropy production can be proved to be an always positive quantity which only vanishes at equilibrium. For quantum systems the Shannon entropy is replaced by the von Neumann entropy of the system $S = -\mathrm{tr}_{\mathrm{S}}\rho_{\mathrm{S}} \ln \rho_{\mathrm{S}}$ and a very similar formulation holds as long as the quantum system is weakly coupled to its bath and described by a Markovian quantum master equation [Spohn and Lebowitz, 2007, Breuer and Petruccione, 2002]. The heat exchanged with the bath is then expressed in terms of the system Hamiltonian by integrating $\dot{Q} \equiv \mathrm{tr}_{\mathrm{S}} H_{\mathrm{S}} \dot{\rho}_{\mathrm{S}}$. An attempt to use such an expression for the entropy production for the QBM model was made in [Nieuwenhuizen and Allahverdyan, 2002] but with non satisfactory results, since a negative entropy production rate was obtained for non-vanishing system-bath coupling strength. A more satisfactory definition of entropy production has been recently introduced by Esposito, Lindenberg and Van den Broeck [Esposito et al., 2010] (denoted here by ELB) in the form $\Delta_{\mathrm{i}} S = \Delta S - Q/T$, where the heat is now defined as minus the energy change in the bath ($\dot{Q} \equiv -\mathrm{tr} H_B \dot{\rho}_B$). This quantum entropy production is positive definite even for finite bath sizes, notwithstanding recurrences. This definition applies on the assumption that the central system and the bath have uncorrelated density matrices at the initial time.

In this work, we compare this definition of entropy production $\Delta_{\mathrm{i}} S$ with a new definition $\Delta_{\mathrm{i}} S^{\mathrm{P}}$, inspired by the one introduced in [Breuer and Petruccione, 2002]

in the context of Markovian master equations. The corresponding heat definition is expressed in term of the averaged change of an effective Hamiltonian which reduces to the system Hamiltonian H_S in the weak-coupling limit. We evaluate analytically both expressions of the entropy production for the QBM model and evaluate their difference. We consider only Gaussian initial conditions, both for the bath and for the central oscillator, what guarantees that the density matrix remains Gaussian at all times. We find that $\Delta_{\mathrm{i}}S$ is positive definite but can present oscillations while $\Delta_{\mathrm{i}}S^{\mathrm{P}}$ is positive definite and has a positive time derivative only in the Markovian high-temperature or weak-coupling limits. The difference between the two definitions considerably depends on the coupling. We also study the behavior of the entropy production for finite-size thermal baths, where Poincaré recurrences characterize the time evolution of the system. The convergence towards a continuous relaxing behavior is studied as a function of the system size. It turns out that a Lorentzian, rather than uniform, sampling of oscillation frequencies of the bath guarantees a better convergence. Finally the evolution the von Neumann entropy of the bath is studied. It is found that, for fixed initial conditions, its asymptotic value does not depend on the coupling in the classical limit while it does in the quantum regime. However, in both cases the Kullback-Leibler divergence between the density matrix of the bath at time t and at canonical equilibrium depends considerably on the coupling, making the usual approximation of the ideal bath problematic.

In the case of two or multiple reservoirs, a way to split the entropy production $\Delta_{\mathrm{i}}S$ into an adiabatic $\Delta_{\mathrm{a}}S$ and a non-adiabatic contribution $\Delta_{\mathrm{na}}S$ has been introduced, in analogy with the context of Markovian master equations [Esposito and Van den Broeck, 2010a,Esposito and Van den Broeck, 2010b]. The rate of the adiabatic term is the only surviving after the relaxation of the central system to the steady state, when it is determined from the constant heat current from one bath to the other. Interestingly our definition establishes a condition for the positivity of both the adiabatic and non-adiabatic terms, which is satisfied in the Markovian limit of the QBM model. Nothing can be said in general about the sign of rates. Finally we found analytical expressions of entropy flow rate $\Delta_{\mathrm{e}}S$ for the QBM model with two baths, which would enable in a future work a detailed study of the adiabatic and non-adiabatic terms.

Outline

An introductory discussion over general aspects of equilibrium thermodynamics, non-equilibrium Markovian dynamics, problems for the definition of thermodynamic equilibrium of small open quantum systems, and aspects of quantum non-equilibrium are reported in chapter 1. In chapter 2 the different definitions of the

entropy production are spelled out, along with the general protocol adopted. Definition of entropy production with a single reservoir is detailed also in the case of an external driving which tunes the parameters of the central system Hamiltonian and the interaction term. In chapter 3 the Quantum Brownian Motion model is introduced and solved. Initial conditions are specified in 3.1 and the evolution of the system is described in section 3.2 via its Wigner quasi-distribution function. The approach to the thermodynamic limit is described in section 3.3. Explicit expressions of the definitions of entropy for our model are reported in chapter 4. Chapter 5 is devoted to a study of the model with a finite-sized bath, where Poincaré recurrences characterize its behavior. A discussion of the bath entropy, correlation entropy and of the distance of the bath density operator from its canonical form is reported in section 6. The Quantum Brownian Motion model with two baths is introduced and solved and it is found the analytical expression for the entropy production rate in chapter 7. In chapter 7.3 we conclude and summarize our results. A few technical details are relegated in several appendices.

Chapter 1

Classical and quantum aspects of thermodynamics

1.1 Equilibrium and irreversibility

Classical equilibrium statistical thermodynamics, as described exhaustively in several textbooks, is fundamentally based on the possibility to describe a closed system with Hamiltonian H via a probability distribution in the space of configurations C of the canonical form

$$P^{\mathrm{eq}}[C] = e^{-\beta H[C]}/Z, \qquad Z = \int \mathcal{D}[C]\, e^{-\beta H[C]}, \tag{1.1}$$

with Boltzmann factor $\beta = 1/k_B T$. Once the energy U and the Shannon entropy S are defined as functionals of the equilibrium probability distribution $P^{\mathrm{eq}}[C]$

$$U = \int \mathcal{D}[C]\, H[C]\, P^{\mathrm{eq}}[C], \tag{1.2}$$

$$S = -\int \mathcal{D}[C]\, P^{\mathrm{eq}}[C] \ln P^{\mathrm{eq}}[C], \tag{1.3}$$

where $H[C]$ is the energy of the configuration C, $P^{\mathrm{eq}}[C]$ is found by minimizing the free energy potential $F = U - TS$. This means also that, by expressing the free energy as $F = -(1/\beta)\ln Z$, 'thermostatic' quantities like energy and entropy can be obtained from F:

$$S = \beta^2 \frac{\partial F}{\partial \beta}, \quad U = F + \beta \frac{\partial F}{\partial \beta}. \tag{1.4}$$

This is actually an axiomatic approach starting from a variational principle, which can also be equivalently formulated in terms of the maximization of the

statistical entropy S, with the average energy U fixed at a constant value. The principle of maximum entropy, introduced by Jaynes [Jaynes, 1957], is based on an information theoretical interpretation of entropy, as measure of lack of information, or degree of disorder. From the measure of uncertainty one should be able to make a statistical inference of some quantities in the most unbiased way, given the certain or probabilistic knowledge of other quantities (see also [Balian, 1999]). By choosing to maximize entropy means to retain all the available information and discarding any other irrelevant and biased information, which would decrease the value of S.

On the other hand Shannon entropy S has the same properties which second law postulates for thermodynamic entropy. It is additive in the case the subsystem probability distribution factorize, it is concave, and extensive, as shown for a wide class of inter-particle interactions, in the limit of a large number of particles [Ruelle, 1969, Lieb, 1976, Thirring, 1981]. Its identification with the thermodynamic entropy is obtained by taking into account the first law of thermodynamics

$$\mathrm{d}U = \delta Q + \delta W. \tag{1.5}$$

In fact, an infinitesimal change of the parameters defining H implies that the energy change $\mathrm{d}U$ can be written as the sum of the work

$$\delta W = \int \mathcal{D}[C]\, \mathrm{d}H[C]\, P^{\mathrm{eq}}[C], \tag{1.6}$$

and the heat

$$T\mathrm{d}S = \delta Q = \int \mathcal{D}[C]\, H[C]\, P^{\mathrm{eq}}[C]\, \mathrm{d}\ln P^{\mathrm{eq}}[C]. \tag{1.7}$$

Therefore, due to the second law of thermodynamics, the quantity $\mathrm{d}S = \delta Q/T$ has to correspond to the change of the thermodynamic entropy, since δQ is an exact differential. The same considerations can extended to the Von Neumann entropy in the quantum case [Balian and Balazs, 1987], even when the operators contained in the Hamiltonian do not commute. In this case we have a trace over the system Hilbert space of states in place of the integral over the space of configurations, and averages of any operator are done by using a density matrix operator [Breuer and Petruccione, 2002].

Physical reliability of $P^{\mathrm{eq}}[C]$ is based on the fact that fluctuations of intensive variables are of order $O(N^{-1/2})$, if N is the number of particles which constitute the system, so that in the thermodynamic limit $N \to \infty$ they are vanishingly small. The same probability distribution can be derived with the microcanonical approach for an open system in weak contact with a thermal reservoir both in the classical [Peliti, 2011] and the quantum case [Balian and Balazs, 1987]. Basic

assumptions are that in the thermodynamic limit the magnitude of the interaction of the system with the reservoir is negligible respect to the system energy, and at the same time the energy of the system is negligible respect to the energy of the reservoir.

The second law of thermodynamics, or more precisely thermostatistics, refers to the growth of entropy for an isolated system which passes from a state of local equilibrium at time t_0 to a state of global equilibrium at a later time t_1 [Callen, 1985]. This transition can happen in the thermodynamic regime, namely by passing through successive states of local equilibrium or in a non-thermodynamic regime, as in the case of an explosive chemical reaction, a shock wave etc. Entropy production is intimately related to the limited subjective description of statistical mechanics [Balian, 1999, Balian, 2005], which explains the paradox of irreversibility by Poincaré. Actually the concept of entropy of a system has to do with the choice of a set of variables relevant to the observer, which often correspond to coarse-grained measurable quantities. The observer realizes the correspondence between a set of macroscopic quantities $\mathcal{A}_i$ and the average values $\langle A \rangle_i$ assumed by a set of observables A_i. This description is incomplete since it does not include all the microscopical features of the system, which are disregarded when the Von Neumann entropy is maximized. The result of maximization is the relevant density matrix at initial time

$$\rho_{\mathrm{R}}(t_0) = \exp\left[-\psi - \sum_i \gamma_i A_i\right], \tag{1.8}$$

which has the same Gibbsian form of (1.1), where ψ is a normalization factor and the parameters γ_i are obtained by imposing $\langle A_i \rangle = \mathrm{tr}\, A_i \rho_{\mathrm{R}}(t_0) = \mathcal{A}_i$. Let us assume now that density operator $\rho_{\mathrm{R}}(t_0)$ coincides with the initial density operator for the evolution. The complete dynamics is totally reversible, due to the unitary evolution of observables in the quantum case

$$i\hbar \frac{\mathrm{d}O}{\mathrm{d}t} = [H, O]\,, \tag{1.9}$$

or analogously due to the time reversibility of the Hamiltonian equations in the classical case. Then Von Neumann entropy is conserved when calculated with the unitary-evolved density operator $\rho(t)$, but generally loses its initial Gibbsian form (1.8). This implies that by definition the relevant entropy $S_{\mathrm{R}}(t)$ has to be bigger, because it is calculated at each time by the maximum entropy principle, according to the new values $\mathcal{A}_i(t) = \mathrm{tr} A_i \rho(t)$ assumed by the relevant observables.

The increase registered in S_{R} has to correspond to a flow of information towards the irrelevant degrees of freedom. This can be formalized by using the projection method of Nakajima and Zwanzig [Zwanzig, 2001], decomposing the

Liouville equation for the evolution of the density operator $\rho(t)$ into an equation for the projection of $\rho_{\mathrm{R}}(t) = \mathcal{P}\rho(t)$ over the relevant part, coupled with the equation for the projection over the irrelevant part $(1 - \mathcal{P})\rho(t)$ [Balian, 1999]. The equation for $\rho_{\mathrm{R}}(t)$ and correspondingly that for the relevant quantities $\mathcal{A}_i(t)$, contains a term which is due to the direct interaction between the relevant observables and another which describes the effect of the coupling with the irrelevant ones via a memory kernel $\mathcal{M}(t, t')$. The latter characterizes also the dissipation, namely the time derivative of the relevant entropy $S_{\mathrm{R}}(t)$ which results as

$$\frac{\mathrm{d}S_{\mathrm{R}}}{\mathrm{d}t} = \sum_i \gamma_i(t) \int_{t_0}^{t} \mathrm{d}t' \mathrm{tr} A_i \mathcal{M}(t, t') \mathcal{P}\rho(t'), \tag{1.10}$$

where the $\gamma_i(t)$'s are the parameters which define the relevant density matrix at time t. Term $\mathcal{M}(t, t')$ has a memory effect, related to the history of the coupling with the irrelevant variables and to the initial relevant density matrix.

Even if relevant entropy is by definition bigger than the initial Von Neumann entropy, its time derivative can be negative and a temporary come-back of information from the irrelevant variables is possible, due to the non-Markovian character of (1.10). If the choice of the relevant variables is such that the irrelevant ones evolve rapidly so to interfere destructively, the memory time over which $\mathcal{M}(t, t')$ is relevant is short respect to the characteristic time of variation of $\rho_{\mathrm{R}}(t)$. Then one realizes the so-called Markovian approximation and obtains a local time-independent evolution, by replacing $\rho_{\mathrm{R}}(t')$ with $\rho_{\mathrm{R}}(t)$ and t_0 with $-\infty$ in (1.10) [Balian, 1999]. Due to short memory, any $\rho_{\mathrm{R}}(t)$ can be considered an initial density operator, what means that at each time relevant entropy S_{R} has to increase, with an irreversible loss of information.

The thermodynamic irreversible regime, corresponds to the Markovian dynamics. It relies on the possibility to coarse-grain the description of the total system in a set of subsystems, to which it is possible to assign a set of observables with a defined slow-varying average value. This is possible only if the interaction between the subsystems is weak. In order to guarantee irreversibility it is fundamental that all slow degrees of freedom be included, with a sharp time-scale separation respect to the fast, irrelevant ones.

1.2 Entropy production in the classical Markovian regime

We consider here an open system in contact with one or more reservoirs. Its description can be reduced to a generalized Langevin equation, characterized by a non-local damping kernel and a colored noise, where apart from the damping, any

force acting on the system is completely independent from the noise, while in the strong-coupling limit one should consider also a renormalization of the effective Hamiltonian of the central system.

In the thermodynamic limit and weak coupling with the reservoir, dynamics of the open system is often supposed to become Markovian, since the total effect of the bath degrees of freedom is suppressed due to destructive interference. Then by neglecting what happens at short time scales, the effect of the reservoirs can be schematized by white noise and local damping. Due to its economical character, this formalism has plenty of applications in condensed matter physics, quantum optics, atomic physics and chemistry [Klimontovich, 1995, Gardiner and Zoller, 2004, Gardiner, 1985]. The most important instrument to describe classical non-equilibrium thermodynamics of these systems is the Fokker Plank equation for the evolution of the probability distribution [Risken, 1989, Gardiner, 1985]. Here relation with equilibrium thermodynamics is readily found. In fact the stationary probability distribution assumes a Gibbsian form, even if, when the Hamiltonian of the central system is not quadratic, the temporal analytical solution is not a simple matter [Lindenberg and West, 1990].

Stochastic description is adapt to investigate thermodynamics properties deep into the non-equilibrium region. In recent years it has been possible to derive exact thermodynamics statements for small systems with significant fluctuations. These are based on the possibility to describe relevant thermodynamic quantities of the single particle at the level of its trajectory in phase space. A large number of Fluctuation Theorems (FT) adapt to the description of diverse physical configurations has been derived. They express universal properties of the functional probability distributions for work, heat or entropy. FT's are fundamentally based on the parity relation existing between the functional $S([x])$ associated to the trajectory $[x]$ of a relevant physical quantity and the functional $S^\dagger\left[x^\dagger\right]$ associated to some conjugate dynamics for the same physical quantity

$$S^\dagger\left[x^\dagger\right] = \epsilon S([x]), \tag{1.11}$$

where $\epsilon = \pm 1$ [Seifert, 2005].

For example, we briefly recall here the Crooks' FT [Crooks, 2000], which is valid for a system in contact with a reservoir at temperature $T = 1/(k_B\beta)$ and subject to a time dependent potential $V(q, \lambda_t)$

$$\frac{P_F(W_{diss})}{P_R(-W_{diss})} = e^{\beta W_{diss}}. \tag{1.12}$$

It expresses a relation between the probability of having a dissipated work $W_{diss} = W - \Delta F$ along the forward (F) dynamics and the probability for having negative-dissipated work $-W_{diss}$ along the time-reversed (R) dynamics. Free energy difference ΔF is evaluated according to the equilibrium distribution corresponding to

the initial and final values of the driving parameter λ_t. Consequences of eq. (1.12) are that one can experimentally determine the value of ΔF due to the splitting between the forward and reversed probability distributions. Furthermore, there is the possibility of violating the second law along given trajectories, even if on average it still holds, since $\langle W \rangle \geq \Delta F$ [Jarzynski, 1997b, Jarzynski, 1997a]. Anyway the probability of these trajectories decreases by enlarging the size of the system, when the probabilities distributions get peaked in correspondence of their the point of maximum.

In the case of a system characterized by discrete states, classical non-equilibrium Markovian processes can be formulated via the following master equation

$$\dot{p}_m(t) = \sum_{m',\nu} W^{(\nu)}_{m,m'}(\lambda_t) p_{m'}(t), \tag{1.13}$$

where $p_m(t)$ are the occupation probabilities of the different states m, and the transitions rates $W^{(\nu)}_{m,m'}(\lambda_t)$ between the states can be related to different mechanisms ν, as for example reservoirs at different temperatures, and depend explicitly on time via the parameter λ_t, if an external force is exerted. Being able to separate the transition probabilities related to different reservoirs, implies they are weakly coupled with the central system.

The time derivative of the Shannon entropy can be split into two contributions,

$$\dot{S}(t) = -\sum_m \dot{p}_m \ln p_m = \dot{S}_e(t) + \dot{S}_i(t), \tag{1.14}$$

the entropy flow rate

$$\dot{S}_e(t) = \sum_{m,m',\nu} W^{(\nu)}_{m,m'}(\lambda_t) p_{m'}(t) \ln \frac{W^{(\nu)}_{m,m'}(\lambda_t)}{W^{(\nu)}_{m',m}(\lambda_t)}, \tag{1.15}$$

and the positive entropy production rate

$$\dot{S}_i(t) = \sum_{m,m',\nu} W^{(\nu)}_{m,m'}(\lambda_t) p_{m'}(t) \ln \frac{W^{(\nu)}_{m,m'}(\lambda_t) p_{m'}(t)}{W^{(\nu)}_{m',m}(\lambda_t) p_m(t)}. \tag{1.16}$$

Different channels ν can be made correspond to the exchange of heat with different reservoirs. The equilibrium distribution $p^{\mathrm{eq}}(\lambda_t, \nu)$, which satisfies the condition of local detailed balance,

$$W^{(\nu)}_{m,m'}(\lambda_t) p^{\mathrm{eq}}_{m'}(\lambda_t, \nu) = W^{(\nu)}_{m',m}(\lambda_t) p^{\mathrm{eq}}_m(\lambda_t, \nu), \tag{1.17}$$

namely the stationary distribution in the case there is only the reservoir ν, is a canonical distribution $p^{\mathrm{eq}}_m(\lambda_t, \nu) \propto \exp -\beta^{(\nu)} \epsilon_m(\lambda_t)$ where $\beta^{(\nu)}$ is the Boltzmann coefficient associated to the reservoir ν. This assumption is a consequence of weak-coupling between system and each reservoir. This gives a physical meaning to

the mathematics which is derived from (1.13). In fact in this case the entropy flow rate can be written as the sum of heat flows over the temperatures of the respective baths.

$$\dot{S}_e(t) = \sum_\nu \beta^{(\nu)} \dot{Q}^{(\nu)}(t), \quad \dot{Q}^{(\nu)}(t) = \sum_{m,m'} J^{(\nu)}_{m,m'}(t)\epsilon_m(\lambda_t), \tag{1.18}$$

where we used the probability fluxes

$$J^{(\nu)}_{m,m'} = W^{(\nu)}_{m,m'}(\lambda_t)p_{m'}(t) - W^{(\nu)}_{m',m}(\lambda_t)p_m(t). \tag{1.19}$$

One can identify also the work due to the changing driving parameter λ_t from the first principle of thermodynamics [Esposito and Van den Broeck, 2010b].

Detailed balance condition (1.17) is related to the assumption that each bath ν relaxes at each time infinitely fast at its equilibrium. Moreover since the baths are assumed to stay at equilibrium, no irreversible process takes place within them, so that the total entropy production rate has to coincide with $\dot{S}_i(t)$ and consequently $\dot{S}_e(t) = -\dot{S}_r(t)$, where $\dot{S}_r(t)$ is the entropy increase in the reservoir.

Interestingly the entropy production rate can be split into the sum of two contributions which are both positive, the adiabatic $\dot{S}_a$ and the non-adiabatic $\dot{S}_{\mathrm{na}}$ [Esposito and Van den Broeck, 2010b]. The first one is

$$\dot{S}_{\mathrm{a}}(t) = \sum_{m,m',\nu} W^{(\nu)}_{m,m'}(\lambda_t)p_{m'}(t) \ln \frac{W^{(\nu)}_{m,m'}(\lambda_t)p^{\mathrm{st}}_{m'}(t)}{W^{(\nu)}_{m',m}(\lambda_t)p^{\mathrm{st}}_m(t)}, \tag{1.20}$$

where $p^{\mathrm{st}}_m(\lambda_t)$ is the stationary probability distribution:

$$\sum_{m'} W_{m,m'}(\lambda_t)p^{\mathrm{st}}_{m'}(\lambda_t) = 0. \tag{1.21}$$

The second one, which does not contains any explicit reference to the different mechanisms ν

$$\dot{S}_{\mathrm{na}}(t) = -\sum_m \dot{p}_m(t) \ln \frac{p_m(t)}{p^{\mathrm{st}}_m(\lambda_t)}, \tag{1.22}$$

is due to the relaxing of the probability distribution $p_m(t)$ to the stationary one $p^{\mathrm{st}}_m(\lambda_t)$. In case the driving on λ is sufficiently slow to let a fast equilibration of $p_m(t)$ to $p^{\mathrm{st}}_m(\lambda_t)$ this term vanishes, so that the transformation can be effectively defined as 'adiabatic', since the system passes through successive states of equilibrium. The positivity of the three rate terms $\dot{S}_i(t)$, $\dot{S}_{\mathrm{a}}(t)$ and $\dot{S}_{\mathrm{na}}(t)$ derives from the conservation of probability $\sum_{m,\nu} W^{(\nu)}_{m,m'} = 0$, stationarity condition (1.21) and to the Jensen inequality inequality $-\ln x \geq 1 - x$. Moreover three fluctuation theorems hold for the corresponding integral quantities $\Delta_{\mathrm{i}}S(t)$, $\Delta_{\mathrm{a}}S(t)$ and $\Delta_{\mathrm{na}}S(t)$ [Esposito and Van den Broeck, 2010a].

In general problems arise experimentally when in a non-Markovian dynamics it is not possible to access to all slow variables. Even if identification of physical quantities entering the first law is independent from the Markovian assumption, the identification of entropy production is often not possible. It is in fact fundamental that for fixed parameters a thermodynamic equilibrium will be reached for an arbitrary initial distribution of the slow variables. Generalized Langevin equation guarantees this, as far as the memory kernel determines the correlations of the colored noise [Zamponi et al., 2005, Speck and Seifert, 2007, Mai and Dhar, 2007, Hasegawa, 2011].

1.3 Quantum difficulties

In the quantum description other some problems due to the presence of quantum correlations. In particular, when looking at nanoscale-sized systems coupled to quantum environments, the interaction with the reservoir is often no longer negligible respect to the system energy. This means that while the axiomatic Gibbsian description do applies also to closed quantum systems, it is not generally possible also for open quantum systems. Nowadays plenty of experimental situations exist which show the inconsistencies of a Gibbsian weak-coupling limit description. We mention for example super-conductive regions connected by Josephson junctions in the over-damped regime [Koch et al., 1980], spin dynamics in quantum dots [Cohen and Kottos, 2004] and optical excitation for molecular wave functions [Suominen et al., 1992].

Consider a generic Hamiltonian of a closed system formed by an open system S interacting with a reservoir B, via an interaction term H_{I}

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}}, \tag{1.23}$$

and its corresponding Gibbsian equilibrium density operator,

$$\rho^{\mathrm{eq}} = \frac{e^{-\beta H}}{Z}, \quad Z = \mathrm{tr}\, e^{-\beta H}, \tag{1.24}$$

The reduced density operator of the system S

$$\rho_{\mathrm{S}}^{\mathrm{eq}} = \mathrm{tr}_{\mathrm{B}} \rho^{\mathrm{eq}}, \tag{1.25}$$

has not in general a Gibbsian form.

A reference Hamiltonian model for an open system coupled to a reservoir is the Quantum Brownian Motion (QBM) introduced by Ullersma [Ullersma, 1966]: an harmonic oscillator is coupled to a bath of harmonic oscillators via a bilinear term depending on the position operators. Due to the linearity of the model it is

analytically solvable. Explicit calculations are made in the thermodynamic limit by using a realistic continuum of bath modes which is realized via a Drude-like Ullersma's coupling strength [Ullersma, 1966, Haake and Reibold, 1985]. It was shown that for this model the occupation probability $e^{-\beta E_n}/Z$ of the eigenstates $|n\rangle$ of the quadratic Hamiltonian $H_{\rm S}^{\rm eq}$ defining the equilibrium density matrix

$$\rho_{\rm S}^{\rm eq} = \frac{e^{-\beta H_{\rm S}^{\rm eq}}}{Z_{\rm S}^{\rm eq}}, \quad Z_{\rm S}^{\rm eq} = {\rm tr}_{\rm S} e^{-\beta H_{\rm S}^{\rm eq}}, \tag{1.26}$$

does not vanish at zero temperature [Grabert et al., 1984], due to the entanglement between system and reservoir [Breuer and Petruccione, 2002]. Then at $T = 0$ system S is not in the ground state of the effective Hamiltonian $H_{\rm S}^{\rm eq}$, and consequently, while the total Von Neumann entropy vanishes, the entropy of the reduced system S

$$S = -{\rm tr}\rho_{\rm S}^{\rm eq} \ln \rho_{\rm S}^{\rm eq}, \tag{1.27}$$

does not [Allahverdyan and Nieuwenhuizen, 2002]. This appears to be in contrast with the third law of thermodynamics. Various definition for energy, entropy, and heat have actually been introduced for the equilibrium thermodynamics description of an open quantum system strongly interacting with a thermal bath. Each of them traces its roots in classical statistical thermodynamics or have a definite physical sense, nonetheless some discrepancies emerge which prevent an univocal description. All differences and problems vanish only in the weak-coupling limit.

1.3.1 Violation of the second law?

A relevant aspect of the QBM model at $T = 0$ is the possibility of violating the Clausius inequality $\delta Q \leq T{\rm d}S$: since the bath is not in its ground state, its energy could be lowered by a positive transfer of heat $\delta Q \geq 0$ to the central system. A positive exchange of heat at zero temperature can actually be observed for a quasi-static change of parameters as the mass or the oscillation frequency of the central oscillator, from which both $H_{\rm S}$ and $\rho_{\rm S}^{\rm eq}$ depend. In fact by defining the energy as

$$U = \langle H_{\rm S} \rangle_{\rm eq} = {\rm tr}\rho_{\rm S}^{\rm eq} H_{\rm S}, \tag{1.28}$$

where $\rho_{\rm S}^{\rm eq}$ is given in (1.26), according to the first law of thermodynamics

$${\rm d}U = đQ + đW, \tag{1.29}$$

an infinitesimal variation of U can be split into a component due to the change of $\rho^{\rm eq}$ (1.24) identified as the heat $đQ$,

$$đQ = \left\langle H_{\rm S} \frac{{\rm d}\ln \rho_{\rm S}^{\rm eq}}{{\rm d}\alpha} \right\rangle_{\rm eq} {\rm d}\alpha, \tag{1.30}$$

plus one associated to the averaged change of H_S, the work $đW$:

$$đW = \left\langle \frac{dH_S}{d\alpha} \right\rangle_{eq} d\alpha, \tag{1.31}$$

where α represents the mass or frequency parameter. It turns our that a variation of each of the parameters appearing H_S can be made so that $đQ \geq 0$ [Allahverdyan and Nieuwenhuizen, 2000, Hilt and Lutz, 2009]. A violation of the Clausius inequality seems to hold also at temperature close to zero, where one can show that for a finite variation of the parameters [Hilt et al., 2011]

$$\Delta Q^{(\alpha)} \geq \Delta S^{(\alpha)}, \tag{1.32}$$

where $\Delta S^{(\alpha)}$ is the difference of the Von Neumann entropy (1.27) of the central system calculated with the final value α_f and the initial value α_i of the variation protocol. Violations disappear in the high-temperature, weak-coupling limit. Another relevant consequence of having the central oscillator with an energy $\langle H_S \rangle_{eq} > \langle H_S \rangle_0$ is that one could make work out of it by fishing out the central oscillator, and to be able to do a cyclic extraction of energy from a single reservoir. This would be a violation of the Thompson formulation of the second law [Ford and O'Connell, 2006], [Kim and Mahler, 2007].

A fundamental observation in order to resolve these paradoxes is the fact that the Clausius inequality presupposes an initial Gibbsian state [Kubo, 1968, Hilt et al., 2011]. Validity of Clausius and Thompson formulations is preserved in the QBM model by considering the work W^c which is needed to couple the central oscillator to the bath, acting before the quasi-static change of the parameters of H_S. The principle of minimum work [Landau and Lifshits, 1958] states that the minimum work required to change the thermodynamic state of a system is given by the difference of the final and initial-state Helmoltz free energies. Accordingly one can express the coupling work as

$$W^c = \int_0^\eta d\eta' \frac{dH_I}{d\eta'} \rho^{eq}(\eta', \alpha_i) = F(\eta, \alpha_i) - F(0, \alpha_i), \tag{1.33}$$

where η is the linear coupling parameter through which the interaction inside H_I (1.23) is tuned [Hilt et al., 2011]. Here we have the total coupled-system free energy

$$F(\eta, T, \alpha_i) = -\frac{1}{\beta} \ln \mathrm{tr} e^{-\beta(H_S(\alpha_i) + H_B + H_I(\eta))}, \tag{1.34}$$

which for $\eta = 0$ reduces to the sum of the uncoupled bath and central system free energies.

The heat exchanged in the coupling process is $Q^{(c)} = \Delta U^{(c)} - W^{(c)}$, with $\Delta U^{(c)} = U(\eta, \alpha_i) - U(0, \alpha_i)$ the difference of system energy (1.28). Then, By composing

the coupling process and the adiabatic change of the parameters of H_S (1.32), it turns out that the Clausius inequality is now fulfilled [Hilt et al., 2011]

$$Q^{(c)} + Q^{(\alpha)} \leq \Delta S^{(c)} + \Delta S^{(\alpha)}, \tag{1.35}$$

where $\Delta S^{c} = S(\eta, \alpha_i) - S(0, \alpha_i)$ is the change of entropy (1.27) due to the coupling. Moreover one has that

$$W^{(c)} \geq \Delta U^{c}, \tag{1.36}$$

so that the minimum work which occurs to couple the central system to the reservoir is greater than the maximum useful work which can be extracted from the central oscillator in the decoupling process [Kim and Mahler, 2007], which actually coincides with the change of its internal energy. Their difference is highest at $T = 0$ and by growing the temperature asymptotically vanish.

An attempt to overcome the above-seen difficulties is to introduce an effective description for the central system, which opportunely includes interactions with the environment. This proved also useful in [Jarzynski, 2004] to derive a classical non-equilibrium work theorem for a Hamiltonian system formed by the open system strongly coupled with a reservoir, and successively in [Campisi et al., 2009] to extend the validity of the theorem to the quantum case. One introduces the mean field free energy

$$F^{\mathrm{MF}} = -k_B T \ln Z^{\mathrm{MF}}, \quad Z_{\mathrm{S}}^{\mathrm{MF}} = \frac{\mathrm{tr} e^{-\beta H}}{\mathrm{tr}_{\mathrm{B}} e^{-\beta H_{\mathrm{B}}}}, \tag{1.37}$$

where mean field partition function $Z_{\mathrm{S}}^{\mathrm{MF}}$ is the rate of the total Z and the the free-bath Z_{B} partition functions. From F^{MF} mean field energy U^{MF} and entropy S^{MF} are obtained by equations (1.4). One can see that the latter differs from the statistical entropy S (1.27) by the mutual information S_{c}, otherwise called correlation entropy (6.3) [Hörhammer and Büttner, 2008]. In the QBM model with a strictly Ohmic damping, mean field entropy S^{MF} vanishes linearly with the temperature [Hänggi and Ludwig Ingold, 2006], in agreement with third law of thermodynamics. Specific heat $C^{\mathrm{MF}} = \partial U^{\mathrm{MF}}/\partial T$ is actually different from the specific heat $C^{U} = \partial U/\partial T$ derived from energy (1.28) [Hänggi and Ludwig Ingold, 2006, Hänggi et al., 2008]. In fact one gets that the mean field energy instead can by decomposed as

$$U^{\mathrm{MF}} = U + U_{\mathrm{I}}, \quad U_{\mathrm{I}} = \langle H_{\mathrm{I}} \rangle_{\mathrm{eq}} + \langle H_{\mathrm{B}} \rangle_{\mathrm{eq}} - \langle H_{\mathrm{B}} \rangle_{0}\,, \tag{1.38}$$

where $\langle \cdot \rangle_0$ is made with the free bath density matrix $\rho_{\mathrm{B}}^{0} = e^{-\beta H_{\mathrm{B}}}/Z_{\mathrm{B}}$. The difference between U and U^{MF} and correspondingly on the specific heats originates in an averaged interaction term and in the difference of the average bath energy when the total density matrix ρ^{eq} or the free bath density matrix ρ_{B}^{0} are used.

Within the model of a free quantum Brownian particle with Ullersma's coupling strength [Hänggi et al., 2008], it turns out that due to quantum dissipation both the two expressions for the specific heat vanish linearly with the temperature, then satisfying the third law of thermodynamics. Nevertheless they are different both in the high temperature limit, in terms of their quantum corrections, and in the low-temperature quantum limit. Remarkably C^{MF} is negative in the low-temperature regime, if the cut-off of the Ullersma's strength is taken smaller than the damping constant, which corresponds also to negative regions of the density of states.

It is interesting to note that a variation of parameters of H_{S} in (1.38), leads in general to the first law formulation

$$\mathrm{d}U^{\mathrm{MF}} = đW + T\mathrm{d}S^{\mathrm{MF}}, \tag{1.39}$$

where $đW = \mathrm{d}F^{\mathrm{MF}}$ is the usual work due to a variation of the parameters which define the central-system Hamiltonian (1.31), and the mean-field entropy variation

$$T\mathrm{d}S^{\mathrm{MF}} = đQ^{\mathrm{MF}} = đQ + \mathrm{d}U_{\mathrm{I}}, \tag{1.40}$$

contains the heat (1.30) plus the variation of U_{I} (1.38) [Hörhammer and Büttner, 2008]. Then at $T = 0$, one sees that since for the QBM model $\mathrm{d}S^{\mathrm{MF}} = 0$, it has to be also $đQ = -\mathrm{d}U_{\mathrm{I}}$, namely the contribute of the interaction part to the mean field potential is relevant for the fulfillment of the third law.

Violation of the second law (1.32) has been related initially to entanglement between system and reservoir. Remarkably, for the Rubin model, where the bath is made of a chain of oscillators, this has been questioned [Hilt and Lutz, 2009]. There exist a critical temperature T_{c} above which the negativity [Vidal and Werner, 2002], namely the measure of entanglement defined as

$$\mathcal{N}(\rho) = \frac{\| \rho^{T_{\mathrm{S}}} \| - 1}{2}, \tag{1.41}$$

where the trace norm of an operator O is given by $\| O \| = \mathrm{tr}\sqrt{OO^{\dagger}}$, abruptly vanishes even if inequality (1.32) holds for temperatures $T > T_{\mathrm{c}}$. This suggests that mechanisms leading to violation could include aspects of quantum correlations other that entanglement. By the way, recently it has shown that quantum correlation between two subsystems can be present also, when the density matrix is separated [Ollivier and Zurek, 2001].

Effective temperature It could appear improper the use of the temperature of the total system to study the Clausius inequality for a subsystem, as its reduced density operator (1.25) has not in general a Gibbsian form. Actually the presence of the Boltzmann factor β of the total system inside the exponential defining

the reduced density matrix (1.26) is completely arbitrary. In fact the coefficients defining H_S^{eq}, which have a complicate dependence on the coupling constant and on the temperature of the total system, contain also the factor β^{-1} [Grabert et al., 1984]. Due to this arbitrariness one can choose the temperature in an ad-hoc way. In [Kim and Mahler, 2010] the effective mass oscillation frequency and correspondingly the effective temperature $T^*_{\rm eff}$ of the QBM model are defined so that the average of the effective Hamiltonian $H^*_{\rm eff}$ coincides with system energy (1.28):

$$\langle H^*_{\rm eff}\rangle_{\rm eq} = \langle H_S\rangle_{\rm eq}\,. \tag{1.42}$$

The effective Hamiltonian changes but the reduced density matrix and consequently the Von Neumann entropy remain the same. With this choice violations of the second law seen above are eliminated. It can be shown in fact the variation of the effective heat $đQ^*_{\rm eff}$ is related to the variation of the Von Neumann entropy $\mathrm{d}S$ according to the usual thermodynamic expression

$$đQ^*_{\rm eff} = \left\langle H^*_{\rm eff}\frac{\mathrm{d}\ln\rho_S^{\rm eq}}{\mathrm{d}\alpha}\right\rangle_{\rm eq}\mathrm{d}\alpha = T^*_{\rm eff}\mathrm{d}S, \tag{1.43}$$

both for a variation of the parameters of H_S and for a variation of the coupling with the reservoir. Moreover, one can use the partition function of the reduced density matrix (1.26) $Z_S^{\rm eq} = Z^*_{\rm eff}$ to define the effective free energy

$$F^*_{\rm eff} = -k_B T^*_{\rm eff}\ln Z^*_{\rm eff} = U - T^*_{\rm eff}S, \tag{1.44}$$

from which, by deriving respect to $\beta^*_{\rm eff} = (k_B T^*_{\rm eff})$ both entropy S and energy U can be obtained according to the usual relations (1.4).

1.3.2 Quantum aspects of non-equilibrium

Respect to the classical case, the Quantum Langevin Equation is much less known, and it is not straightforward to derive the corresponding quantum master equation, when the potential acting on the central system in non-quadratic. Obviously things get much more complicated when the evolution is non-local and non-Markovian. Actually the stationary density matrix is known only for the harmonic potential, as for the QBM model where the form of the master equation and its solution are exceptionally known even when the damping kernel is non-local. Remarkably, the origin of non-Markovian behavior can be due only to quantum coherences of the bath degrees of freedom. Recently efforts have been directed to characterize the degree of non-Markovian behavior in quantum systems [Breuer et al., 2009] which is based on the time-convolutionless approach for master equations [Breuer and Petruccione, 2002, Breuer and Piilo, 2009].

In the Markovian case it is known that the density operator of the central system satisfies a Quantum Master Equation (QME) in Lindblad form [Breuer and Petruccione, 2002] which can be generally put in the form

$$\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = -i\left[H_{\mathrm{S}}, \rho_{\mathrm{S}}\right] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_{\mathrm{S}} A_k^{\dagger} - \frac{1}{2} A_k^{\dagger} A_k \rho_{\mathrm{S}} - \frac{1}{2} \rho_{\mathrm{S}} A_k^{\dagger} A_k \right), \tag{1.45}$$

where N is the dimension of the Hilbert space of the system, H_{S} is the system Hamiltonian and A_k's are the Lindblad orthogonal operators which provide the coupling of the system to the various decay channels, each with a damping rate γ_k. It is not possible to reduce it in the form of a discrete master equation (1.13) simply by projecting onto the eigenstates of H_{S} due to the non-diagonal terms, namely the coherences which characterize the density operator. This is possible only when the rotative wave approximation hold [Breuer and Petruccione, 2002], namely one has the condition

$$\left[H_{\mathrm{S}}, A_k\right] = -\omega_k A_k, \quad \left[H_{\mathrm{S}}, A_k^{\dagger}\right] = -\omega_k A_k^{\dagger}, \tag{1.46}$$

where the A_k's are eigenoperators of the system Hamiltonian. In this case, by taking the trace with the basis of eigenvectors of H_{S}, the entropy rate can be discretized exactly as in the classical master equation context (1.14), where apart from the entropy flow, one can identify a positive entropy production with positive adiabatic and non-adiabatic contributions, if there is more than one reservoir. On the other hand, with this assumption the stationary density matrix of the central system reduces to the canonical equilibrium one $\rho_{\mathrm{S}}^{\mathrm{eq}} \propto \exp -\beta H_{\mathrm{S}}$ in presence of a single reservoir.

In the quantum realm it is not possible to follow trajectories of the particles in the phase space, due to the uncertainty principle. Anyway fluctuation theorems have been formulated according to different procedures. One of these is the unraveling of the reduced QME for the central system, which can be seen as resulting from a continuous projective measurement on the reservoir. This leads to a continuous positive operator-valued measurement on the system which allows one to construct a trajectory picture in the Hilbert space of states for the central system, where each realization of the continuous measurement leads to a given system trajectory [Breuer and Petruccione, 2002, De Roeck and Maes, 2006, Esposito and Mukamel, 2006]. Some FT's in the counting statistic field are based on the use of the influence functional propagator defined on a Keldish loop as the generating function of the electron counting probability distribution [Nazarov, 2007, Saito and Dhar, 2007], or on a semiclassical scattering approach [Pilgram et al., 2003].

A technique which provides a unified framework to derive FT's has been more recently introduced, where the change of a certain physical observable is determined from a two-point projective measurement [M. Esposito and Mukamel,

2009]. Physically this is the result of the detector-system interaction on the system, so that the detailed modeling of detectors and their dynamics is avoided. This measurement technique has been originally introduced in order to give account of work fluctuation theorems, since work is not an observable [Talkner et al., 2007]. FT's establish the relation between the joint probability $P[a_t, a_0]$ to measure a certain value a_0 of the physical quantity at initial time and conditionally to measure another value a_t at final time, and the probability $P^{\mathrm{TR}}[a_0, a_t]$ to measure the same values in a time-reversed dynamics. By using this symmetry FT's are derived for closed and open systems driven out of equilibrium by an external time-dependent force, and for open systems maintained in a steady state by nonequilibrium boundary conditions.

A brief account of it will be given next, in the context of entropy production for an out-of-equilibrium open system put in contact with a thermal reservoir. On the other hand fluctuation theorems regarding adiabatic and non-adiabatic contributions have not been found yet.

Chapter 2

Entropy production

We consider a central system S coupled to its bath B. The total Hamiltonian is:

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}}. \tag{2.1}$$

We assume to prepare the system and the bath separately, so that no correlation is initially present between them, and to instantaneously switch on the interaction H_{I} at $t = 0$. We also assume that the bath is initially at canonical equilibrium. The density matrix of the total system is therefore of the form

$$\rho(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}(0) \ , \ \rho_{\mathrm{B}}(0) = \rho_{\mathrm{B}}^{\mathrm{eq}} \equiv \frac{\mathrm{e}^{-\beta H_{\mathrm{B}}}}{Z_{\mathrm{B}}} \ , \ Z_{\mathrm{B}} = \mathrm{tr}_{\mathrm{B}} \mathrm{e}^{-\beta H_{\mathrm{B}}}, \tag{2.2}$$

where $\beta = (k_{\mathrm{B}} T)^{-1}$ is the Boltzmann factor and $\rho_{\mathrm{S}}(0)$ and $\rho_{\mathrm{B}}(0)$ are respectively the central oscillator and the bath reduced density matrix. From now on we set $k_{\mathrm{B}} = 1$. The density matrix $\rho_{\mathrm{S}}(t)$ of the system S evolves according to the equation

$$\rho_{\mathrm{S}}(t) = V(t)\rho_{\mathrm{S}}(0) = \mathrm{tr}_{\mathrm{B}}\rho(t), \tag{2.3}$$

with the evolved total density operator

$$\rho(t) = U(t)\rho(0)U^{\dagger}(t), \tag{2.4}$$

where

$$U(t) = \mathrm{e}^{-\mathrm{i}Ht}, \tag{2.5}$$

is the unitary evolution operator in the global system $\mathrm{S} \otimes \mathrm{R}$.

The evolution of the system density matrix (2.3) can be formally written as

$$\dot{\rho_{\mathrm{S}}}(t) = \mathcal{L}(t)\rho_{\mathrm{S}}(t) \ , \ \mathcal{L}(t) = \dot{V}(t)V^{-1}(t), \tag{2.6}$$

where the operator $\mathcal{L}(t)$ in general depends on time. In this case, the evolution operator $V(t)$ may be written as $V(t) = \mathcal{T} \exp\{\int_0^t d\tau \mathcal{L}(\tau)\}$ in which $\mathcal{T}$ indicates the time-ordering operator. The form (2.6) is the starting point to derive convolutionless quantum master equations [Breuer and Petruccione, 2002]. In the Markovian case, $\mathcal{L}(t)$ is time-independent. This typically happens in the thermodynamic limit of the bath for times t larger then the bath correlation time.

2.1 The 'Poised' definition

Let us define the *poised* density matrix $\rho_S^*(t)$ as the solution of

$$V(t)\rho_S^*(t) = \rho_S^*(t). \tag{2.7}$$

Its existence and uniqueness may not always be guaranteed. In the Markovian case, the poised density matrix ρ_S^* becomes constant in time and coincides with the stationary density matrix ρ_S^{st}, defined by $\mathcal{L}\rho_S^{st} = 0$:

$$\rho_S^* = \rho_S^{st}. \tag{2.8}$$

For the QBM model, the poised density matrix is well defined at all times. Its expression is given in equation (4.5) and is derived in A.4.

We can then introduce the following definition of the entropy production:

$$\Delta_i S^P = \left[D(\rho_S(0)||\rho_S^*(t)) - D(\rho_S(t)||\rho_S^*(t))\right], \tag{2.9}$$

where $D(\ldots||\ldots)$ is the Kullback-Leibler divergence, defined by

$$D(\rho||\rho') = \mathrm{tr}\rho\ln\rho - \mathrm{tr}\rho\ln\rho' \geq 0. \tag{2.10}$$

One can prove that the expression (2.9) is positive definite as follows. From equation (2.3) we obtain

$$\begin{aligned} D(\rho_S(t)||\rho_S^*(t)) &= D(V(t)\rho_S(0)||V(t)\rho_S^*(t)) \\ &= D\left(\mathrm{tr}_B U(t)\rho_S(0)\otimes\rho_B(0)U^\dagger(t)||\mathrm{tr}_B U(t)\rho_S^*(t)\otimes\rho_B(0)U^\dagger(t)\right) \\ &\leq D(\rho_S(0)||\rho_S^*(t)), \end{aligned} \tag{2.11}$$

where we have used the property of the Kullback-Leibler divergence

$$D(\rho_1||\rho_2) \geq D(\mathrm{tr}_B\rho_1||\mathrm{tr}_B\rho_2). \tag{2.12}$$

We also introduce the slightly different entropy production

$$\Delta_i S^{Br} = D(\rho_S(0)||\rho_S^{st}) - D(\rho_S(t)||\rho_S^{st}), \tag{2.13}$$

which is also obviously also positive definite in the Markovian case and extends the definition previously proposed by Breuer and Petruccione for weakly coupled systems [Breuer and Petruccione, 2002] where ρ_S^{st} is the canonical distribution expressed in terms of the system Hamiltonian H_S.

In the Markovian case, it follows from (2.11) that the time derivative of $\Delta_i S^P$ as well as that of $\Delta_i S^{Br}$ is also positive [Breuer and Petruccione, 2002, Yukawa, 2001]:

$$\frac{d\Delta_i S^P}{dt} = \frac{d\Delta_i S^{Br}}{dt} = -\lim_{dt\to 0} \frac{D(\rho_S(t+dt)\|\rho_S^{st}) - D(\rho_S(t)\|\rho_S^{st})}{dt} \geq 0. \tag{2.14}$$

This result does not hold in the non-Markovian case where $\mathcal{L}(t)$ depends on t and where $d\Delta_i S^P/dt \neq d\Delta_i S^{Br}/dt$.

It may happen that the stationary density matrix can be expressed as the canonical distribution of some effective Hamiltonian H_S^{eq}. In the weak-coupling limit it corresponds to the system Hamiltonian H_S. Its expression for the QBM model is given in equation (3.53). In such cases, the entropy production (2.13) has a straightforward physical interpretation, since it can be rewritten as

$$\Delta_i S^{Br} = \Delta S - \Delta_e S^{Br}, \tag{2.15}$$

i.e., as the difference between the entropy change ΔS, and the entropy flow $\Delta_e S^{Br}$ identified by the variation of the averaged effective Hamiltonian of the central system:

$$\Delta_e S^{Br} = \beta \Delta \left\langle H_S^{eq} \right\rangle. \tag{2.16}$$

The average of an operator O is defined as $\langle O \rangle = \mathrm{tr}\rho(t)O$ and Δ denotes the difference between the average evaluated at time t and at time 0. We shall see in section 4.1 that in the classical high-temperature limit and in the quantum weak-coupling limit this definition becomes equal to the one used in the usual stochastic thermodynamics setup. In the following, when studying the QBM model for a finite-size bath, where ρ_S^{st} does not exist, and when referring to $\Delta_i S^{Br}$, one should consider the definition (2.15) instead of (2.13). When the bath approaches the thermodynamic limit the two definitions are equivalent.

2.2 The ELB definition

A definition of the entropy production which guarantees its positivity in all cases has been recently introduced by Esposito *et al* [Esposito et al., 2010]. It reads

$$\Delta_i S = D\left(\rho(t)\middle\|\rho_S(t)\otimes\rho_B^{eq}\right). \tag{2.17}$$

This quantity is clearly positive definite and within our assumptions it expresses the second law in the form

$$\Delta_{\rm i} S \;=\; \Delta S \,+\beta\,\Delta\,\langle H_{\rm B}\rangle\,. \tag{2.18}$$

One has in fact, exploiting the conservation of the von Neumann entropy:

$$\begin{aligned} D\left(\rho(t)\|\rho_{\rm S}(t)\otimes\rho_{\rm B}^{\rm eq}\right) &= {\rm tr}\rho(t)\ln\rho(t) - {\rm tr}\rho(t)\ln\rho_{\rm S}(t) - {\rm tr}\rho(t)\ln\rho_{\rm B}^{\rm eq} \\ &= {\rm tr}\rho_{\rm B}^{\rm eq}\ln\rho_{\rm B}^{\rm eq} + {\rm tr}\rho_{\rm S}(0)\ln\rho_{\rm S}(0) - {\rm tr}\rho_{\rm S}(t)\ln\rho_{\rm S}(t) - {\rm tr}\rho_{\rm B}(t)\ln\rho_{\rm B}^{\rm eq} \\ &= \Delta S\,(t) + \left[{\rm tr}\rho_{\rm B}^{\rm eq}\,(-\beta H_{\rm B}) - {\rm tr}\rho_{\rm B}(t)\,(-\beta H_{\rm B})\right]. \end{aligned} \tag{2.19}$$

From (2.18) we observe that the entropy flow

$$\Delta_{\rm e} S \;=\; -\beta\,\Delta\,\langle H_{\rm B}\rangle = \beta(\Delta\,\langle H_{\rm S}\rangle + \Delta\,\langle H_{\rm I}\rangle\,), \tag{2.20}$$

is now identified as the change of the bath energy $H_{\rm B}$ times the inverse temperature β, as usual in equilibrium thermodynamics. It is then proportional to the change of the central oscillator energy plus an interaction term which is discussed in section 4. The time derivative of (2.17) is not generally positive, as we will observe in 4.1.1. Since by (2.16) and (2.20) one has $H^{\rm eq} \to H_{\rm S}$ and $\langle H_{\rm I}\rangle \to 0$, we see that the two definitions coincide in the weak-coupling limit. We note that the positivity of the right-hand-side of (2.18) was also remarked in ref. [Jarzynski, 1999].

2.2.1 Derivation from a Fluctuation Theorem

The positivity of the ELB expression (2.17) for entropy production can actually be derived through a quantum integral fluctuation theorem whose general formulation can be found in [M. Esposito and Mukamel, 2009]. Here we give a brief account of it. Let us introduce the time dependent operator in the total Hilbert space S $\otimes$ B:

$$A(t) = \ln\rho_{\rm S}(t) + \beta H_{\rm B}, \tag{2.21}$$

whose average change between time t and 0 clearly corresponds to ELB entropy production (2.18), when initial conditions (2.2) are assumed. Then we consider the operator

$$R[a_t;a_0] = \ln\frac{P[a_t;a_0]}{P^{\rm TR}[a_0,a_t]}, \tag{2.22}$$

as the logarithm of the ratio of the probability $P[a_t;a_0]$ of measuring the eigenvalue a_0 of $A(0)$ at time 0 and conditionally to measure the eigenvalue a_t of $A(t)$ at time t according to the forward evolution

$$P[a_t;a_0] = |\,\langle a_t|\,U(t,0)\,|a_0\rangle\,|^2\,\langle a_0|\,\rho(0)\,|a_0\rangle\,, \tag{2.23}$$

and the probability $P^{\mathrm{TR}}[a_0, a_t]$ of measuring at initial time a_t and conditionally a_0 at time t for the time reversed TR evolution

$$P^{\mathrm{TR}}[a_0, a_t] = |\langle a_0| U^{\dagger}(t,0) |a_t\rangle|^2 \langle a_0| \rho^{\mathrm{TR}}(0) |a_0\rangle . \tag{2.24}$$

Density operator $\rho^{\mathrm{TR}}(0)$ is the initial condition of the time reversed (TR) dynamics. The eigenvalues of $A(t)$ are $a_t = \lambda_t - \beta E_{\mathrm{B}}$, where λ_t is a time-dependent eigenvalue of $\ln \rho_{\mathrm{S}}(t)$, and E_{B} of H_{B} with eigenvectors respectively in the bath B Hilbert space. For brevity we have not considered here degenerate states, but the result is equivalent. One immediately sees that

$$\left\langle e^{-R} \right\rangle = \sum_{a_t, a_0} P[a_t; a_0] e^{-R[a_t; a_0]} = \sum_{a_t, a_0} P^{\mathrm{TR}}[a_0; a_t] = 1, \tag{2.25}$$

and due to the Jensen inequality $\left\langle e^{X} \right\rangle \geq e^{\langle X \rangle}$ one gets

$$\langle R \rangle = \sum_{a_t, a_0} P[a_t; a_0] R[a_t; a_0] \geq 0. \tag{2.26}$$

In order to recover expression (2.17) for ELB entropy production, one has to assure that the initial conditions for the forward and reversed dynamics fulfill the following commutation properties

$$[A(0), \rho(0)] = 0, \tag{2.27}$$

which is implicit in the choice of $A(t)$ (2.21) when the initial conditions (2.2) are considered, and

$$[A(t), \rho^{\mathrm{TR}}(0)] = 0, \tag{2.28}$$

which is verified by choosing

$$\rho^{\mathrm{TR}}(0) = \rho_{\mathrm{S}}(t) \otimes e^{-\beta H_{\mathrm{B}}} / Z_{\mathrm{B}}. \tag{2.29}$$

In fact, due to equations (2.27) and (2.28), one finds

$$\langle R \rangle = \sum_{a_t, a_0} P[a_t; a_0] \ln \frac{\langle a_0| \rho(0) |a_t\rangle}{\langle a_t| \rho^{\mathrm{TR}}(0) |a_0\rangle} = \mathrm{tr}\rho(0) \ln \rho(0) - \mathrm{tr}\rho(t) \ln \rho^{\mathrm{TR}}(0), \tag{2.30}$$

which gives us back ELB definition (2.17).

2.3 Difference between the two definitions

Since the following identity holds

$$D(\rho(t) || \rho_{\mathrm{S}}^{\mathrm{st}} \otimes \rho_{\mathrm{B}}^{\mathrm{eq}}) = D(\rho(t) || \rho_{\mathrm{S}}(t) \otimes \rho_{\mathrm{B}}^{\mathrm{eq}}) + D(\rho_{\mathrm{S}}(t) || \rho_{\mathrm{S}}^{\mathrm{st}}), \tag{2.31}$$

we find, using (2.17) and (2.13), that the difference between the ELB definition $\Delta_{\rm i}S$ and the Breuer one $\Delta_{\rm i}S^{\rm Br}$ is given by

$$\Delta_{\rm i}S - \Delta_{\rm i}S^{\rm Br} = D(\rho(t)||\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}) - D(\rho_{\rm S}(0)||\rho_{\rm S}^{\rm st}). \tag{2.32}$$

Due to the unitary evolution of the total density operator $\rho(t)$ (2.4,2.5), one can recast the first term of the right hand side of (2.32) in the form

$$D(\rho(t)||\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}) = D(\rho_{\rm S}(0)\otimes\rho_{\rm B}^{\rm eq}||U^\dagger(t)\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}U(t)). \tag{2.33}$$

By inserting this identity into (2.32) and noting that

$$D(\rho_{\rm S}(0)||\rho_{\rm S}^{\rm st}) = D(\rho_{\rm S}(0)\otimes\rho_{\rm B}^{\rm eq}||\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}), \tag{2.34}$$

we obtain

$$\Delta_{\rm i}S - \Delta_{\rm i}S^{\rm Br} = -{\rm tr}\rho_{\rm S}(0)\otimes\rho_{\rm B}^{\rm eq}[\ln U^\dagger(t)\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}U(t) - \ln\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}]. \tag{2.35}$$

Moreover due to the inequality

$$\begin{aligned} &D(\rho_{\rm S}(0)\otimes\rho_{\rm B}^{\rm eq}||U^\dagger(t)\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}U(t)) \\ &\quad\geq D({\rm tr}_{\rm B}\{\rho_{\rm S}(0)\otimes\rho_{\rm B}^{\rm eq}\}||{\rm tr}_{\rm B}\{U^\dagger(t)\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}U(t)\}) \\ &\quad= D(\rho_{\rm S}(0)||{\rm tr}_{\rm B}\{U^\dagger(t)\rho_{\rm S}^{\rm st}\otimes\rho_{\rm B}^{\rm eq}U(t)\}), \end{aligned} \tag{2.36}$$

it follows from (2.35) that

$$\Delta_{\rm i}S - \Delta_{\rm i}S^{\rm Br} \geq -{\rm tr}_{\rm S}\rho_{\rm S}(0)\left[\ln\tilde{V}(t)\rho_{\rm S}^{\rm st} - \ln\rho_{\rm S}^{\rm st}\right], \tag{2.37}$$

where we have introduced the evolution operator for the central system associated to the total adjoint dynamics, implicitly defined by

$$\tilde{V}(t)\rho_{\rm S} = {\rm tr}_{\rm B}\{U^\dagger(t)\rho_{\rm S}\otimes\rho_{\rm B}^{\rm eq}U(t)\}, \tag{2.38}$$

where $\rho_{\rm S}$ is a generic density operator for the system S.

If the operator $\mathcal{L}(t)$ is Markovian, $\tilde{\mathcal{L}}(t) = \dot{\tilde{V}}(t)\tilde{V}^{-1}(t)$ will also be so. If they furthermore have the same stationary state, so that

$$\tilde{V}(t)\rho_{\rm S}^{\rm st} = \rho_{\rm S}^{\rm st}, \tag{2.39}$$

then the right-hand side of (2.37) vanishes and the ELB expression is strictly larger than the Breuer one:

$$\Delta_{\rm i}S - \Delta_{\rm i}S^{\rm Br} \geq 0. \tag{2.40}$$

In A.5 we show that this is indeed the case in the QBM model.

In the following we are going to study these different definitions in the context of the QBM model [Ullersma, 1966, Haake and Reibold, 1985, Caldeira and Leggett, 1983].

2.4 External Driving

We consider here definitions for entropy production in the presence of an external driving which modifies the system S Hamiltonian or the interaction term, such that the total Hamiltonian is written as:

$$H = H_{\rm S}(t) + H_{\rm I}(t) + H_{\rm B}. \tag{2.41}$$

2.4.1 Lutz definition

The following definition of entropy production we call 'Lutz', is the homologous to the 'Breuer' one (2.13) in the absence of an external driving and is an extension to a general Markovian case of that given for the weak coupling limit in [Deffner and Lutz, 2011].

$$\Delta_{\rm i} S^{\rm Lu} = D(\rho_{\rm S}(0)||\rho_{\rm S}^{\rm eq}(0)) - D(\rho_{\rm S}(t)||\rho_{\rm S}^{\rm eq}(t)) - \int_0^t {\rm d}\tau {\rm tr}_{\rm S}\rho_{\rm S}(\tau)\partial_t \ln \rho_{\rm S}^{\rm eq}(\tau), \tag{2.42}$$

where $\rho_{\rm S}^{\rm eq}(t)$ is the density operator satisfying the local stationarity condition $\mathcal{L}(t)\rho_{\rm S}^{\rm eq}(t) = 0$ for the reduced system S dynamics at time t is put in the form

$$\rho_{\rm S}^{\rm eq}(t) = e^{-\beta H_{\rm S}^{eq}(t)} Z_{\rm S}^{\rm eq}(t), \tag{2.43}$$

where $H_{\rm S}^{eq}(t)$ can be in general a complicated function of the coupling and the temperature.

Entropy production (2.42) can be also expressed as:

$$\Delta_{\rm i} S^{\rm Lu} = \beta(W^{\rm Lu}(t) - \Delta F^{\rm Lu}(t)), \tag{2.44}$$

where we have defined the work term

$$W^{\rm Lu}(t) = \int_0^t {\rm d}\tau \left\langle \dot{H}_{\rm S}^{\rm eq}(\tau) \right\rangle_\tau, \tag{2.45}$$

and the out of equilibrium free energy difference

$$\Delta F^{\rm Lu}(t) = \Delta U^{\rm Lu} - T\Delta S, \tag{2.46}$$

with the effective energy change

$$\Delta U^{\rm Lu} = \left\langle H_{\rm S}^{\rm eq}(t) \right\rangle_t - \left\langle H_{\rm S}^{\rm eq}(0) \right\rangle_0. \tag{2.47}$$

In the weak coupling limit one expects that $H_{\rm S}^{\rm eq}(t) = H_{\rm S}(t)$.

Lutz entropy production (2.42) can be shown to be positive in the Markovian dynamics [Deffner and Lutz, 2011], in fact its time derivative is positive

$$\frac{{\rm d}\Delta_{\rm i} S^{\rm Lu}}{{\rm d}t} = -{\rm tr}\dot{\rho}_{\rm S}(t)\ln\rho_{\rm S}(t) + {\rm tr}\dot{\rho}_{\rm S}(t)\ln\rho_{\rm S}^{\rm eq}(t) \geq 0, \tag{2.48}$$

due to the fact that the map $\rho_{\rm S} \rightarrow -{\rm tr}\mathcal{L}(\rho_{\rm S})\ln\rho_{\rm S}$ is a convex functional when superoperator $\mathcal{L}$ has Lindblad form [Breuer and Petruccione, 2002].

2.4.2 ELB definition

By observing that the heat exchange according to the ELB definition in (2.17) can be rewritten as

$$\langle H_{\rm B}\rangle_0 - \langle H_{\rm B}\rangle_t = -\int_0^t {\rm d}\tau\ {\rm tr}\dot{\rho}(t)H_{\rm B} = \int_0^t {\rm d}\tau\ {\rm tr}\left[H_{\rm S}(\tau) + H_{\rm I}(\tau)\right]\dot{\rho_{\rm S}}(\tau), \tag{2.49}$$

where the last equality is due to the fact that for the ciclicity of trace ${\rm tr}\dot{\rho}(\tau)H(\tau) = 0$, one rewrite (2.17) as:

$$\Delta_{\rm i}S = \beta(W(t) - \Delta F(t)), \tag{2.50}$$

where the work $W(t)$ is

$$W(t) = \int_0^t {\rm d}\tau \left\langle \dot{H}_{\rm S}(\tau)\right\rangle_\tau + \left\langle \dot{H}_{\rm I}(\tau)\right\rangle_\tau, \tag{2.51}$$

and the out of equilibrium free energy difference is

$$\Delta F(t) = \Delta U - T\Delta S, \tag{2.52}$$

where the energy change

$$\Delta U = \langle [H_{\rm S}(t) + H_{\rm I}(t)]\rangle_t - \langle [H_{\rm S}(0) + H_{\rm I}(0)]\rangle_0\,. \tag{2.53}$$

The study of ELB expression (2.50) as a function of work and an off-equilibrium free energy, as well as the comparison with the Lutz definition (2.42) goes beyond the scope of this work, where we focus on transient relaxation. It would be interesting the study of these definitions of entropy production from a fast change of parameters to very slow 'equilibrium' transformations.

2.5 Entropy production with multiple reservoirs

Here we are going to consider entropy production in the case of a central oscillator coupled with a 'left' L and a 'right' R reservoirs:

$$H = H_{\rm S} + H_{\rm L} + H_{\rm R} + H_{\rm IL} + H_{\rm IR}; \tag{2.54}$$

The same discussions we make in the following could be easily extended to a general case with n reservoirs. We assume to prepare the system and the two baths separately, and we assume to switch on both the interations $H_{\rm IL}$ and $H_{\rm IR}$ with the two baths at $t = 0$. The two bath are assumed initially at canonical equilibrium at different temperatures $T_{\rm L}$ and $T_{\rm R}$.

$$\rho(0) = \rho_{\rm S}(0)\otimes\rho_{\rm L}(0)\otimes\rho_{\rm R}(0), \quad \rho_{\rm L,R}(0) = \rho^{\rm eq}_{\rm L,R} \equiv \frac{{\rm e}^{-\beta_{\rm L,R}H_{\rm L,R}}}{Z_{\rm L,R}}, \ Z_{\rm L,R} = {\rm tr}_{\rm R,L}{\rm e}^{-\beta_{\rm L,R}H_{\rm L,R}}, \tag{2.55}$$

where $\beta_L = (k_B T_L)^{-1}$ and $\beta_R = (k_B T_R)^{-1}$ are the Boltzmann factors and $\rho_S(0), \rho_L(0)$ and $\rho_R(0)$ are respectively the central oscillator, the left and right bath reduced density matrix.

The evolution of the density matrix is characterized by a time evolution of the kind (2.6). In general the dynamics is non-Markovian, moreover the contribution given by the diffent reservoirs is not separable.

2.5.1 Adiabatic and Non-Adiabatic contributions

In the following we make attempts to split the entropy production into two contributions which we would identify with an adiabatic term, corresponding at late times to the steady state entropy production, and a non-adiabatic term which corresponds to the entropy production due to to the relaxation of the central system to the steady state in analogy with what is seen in the discrete master equation case (1.20,1.22). We use the definition of 'Poised' density operator $\rho_S^*(t)$ (2.7) to introduce the 'Poised' adiabatic and non-adiabatic contributions to ELB entropy production. Then an analogous 'Breuer' definition is introduced by the use of the steady state density operator ρ_S^{ss}.

The evolution of a central-system density operator is defined as:

$$V(t)\rho_S = \mathrm{tr}_B\, U(t)\rho_S \otimes \rho_L^{eq} \otimes \rho_R^{eq} U^\dagger(t), \tag{2.56}$$

for any system density operator ρ_S. In the Markovian case, the poised density matrix reduces to steady state density matrix $\rho_S^*(t) = \rho_S^{ss}$, which satisfies $\mathcal{L}\rho_S^{ss} = 0$.

ELB entropy production (2.17) has a simple generalization in the case of multiple reservoirs connected to the central system [Esposito et al., 2010]. In the case of two baths one has, once initial conditions (2.55) are introduced,

$$\Delta_i S = \Delta S - \Delta_e S = D\left(\rho(t) \middle\| \rho_S(t) \otimes \rho_L^{eq} \otimes \rho_R^{eq}\right), \tag{2.57}$$

so that the entropy flow is now

$$\Delta S_e = -\beta_L \Delta \langle H_L \rangle - \beta_R \Delta \langle H_R \rangle . \tag{2.58}$$

Since the change of entropy for the central system can be rearranged as:

$$\Delta S = D[\rho_S(0) \| \rho_S^*(t)] - D[\rho_S(t) \| \rho_S^*(t)] - \Delta \left\langle \ln \rho_S^*(t) \right\rangle , \tag{2.59}$$

by using the definition of entropy flow (2.57), one sees that entropy production can be decomposed as the sum of an adiabatic

$$\Delta_a S^P \equiv \beta_L \Delta \langle H_L \rangle + \beta_R \Delta \langle H_R \rangle - \Delta \left\langle \ln \rho_S^*(t) \right\rangle , \tag{2.60}$$

and a non-adiabatic term

$$\Delta_{\rm na}S^{\rm P} = D[\rho_{\rm S}(0)||\rho^*_{\rm S}(t)] - D[\rho_{\rm S}(t)||\rho^*_{\rm S}(t)]. \tag{2.61}$$

With exactly the same passages as in (2.11) one can show that:

$$\Delta_{\rm na}S^{\rm P} \geq 0. \tag{2.62}$$

Moreover, in a similar way as done in (2.3), due to the equality

$$D(\rho(t)||\rho^*_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}) = D(\rho(t)||\rho_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}) + D(\rho_{\rm S}(t)||\rho^*_{\rm S}(t)), \tag{2.63}$$

one can express the difference between entropy production and the P non-adiabatic contribution as:

$$\Delta_{\rm i}S - \Delta_{\rm na}S^{\rm P} = -{\rm tr}\rho_{\rm S}(0)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}[\ln U^\dagger(t)\rho^*_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}U(t) - \ln\rho^*_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}]. \tag{2.64}$$

Finally, since the following inequality holds:

$$\begin{aligned} &D(\rho_{\rm S}(0)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}||U^\dagger(t)\rho^*_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}U(t)) \\ &\quad\geq D(\rho_{\rm S}(0)||{\rm tr}_{\rm B}\{U^\dagger(t)\rho^*_{\rm S}(t)\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}U(t)\}), \end{aligned} \tag{2.65}$$

one can assert the following inequality:

$$\Delta_{\rm i}S - \Delta_{\rm na}S^{\rm P} \geq -{\rm tr}_{\rm S}\rho_{\rm S}(0)\left[\ln\tilde{V}(t)\rho^*_{\rm S}(t) - \ln\rho^*_{\rm S}(t)\right], \tag{2.66}$$

where we have introduced the evolution operator for the central system associated to the total adjoint dynamics, implicitly defined by

$$\tilde{V}(t)\rho_{\rm S} = {\rm tr}_{\rm B}\{U^\dagger(t)\rho_{\rm S}\otimes\rho^{\rm eq}_{\rm L}\otimes\rho^{\rm eq}_{\rm R}U(t)\}, \tag{2.67}$$

where $\rho_{\rm S}$ is a generic density operator for the system S.

Then, if one is able to show that the rhs of (2.64) or the rhs of (2.66) are not negative, one gets

$$\Delta_{\rm a}S^{\rm P} \geq 0. \tag{2.68}$$

The rhs of (2.66) actually vanish in the Markovian context of the QBM model with two baths A.5, just like it happens in the case of a single reservoir (2.39), due to the fact that

$$\tilde{V}(t)\rho^{\rm ss}_{\rm S} = \rho^{\rm ss}_{\rm S}, \tag{2.69}$$

which means thus validating inequality (2.68).

Entropy production (2.57) can be split also into the sum of the 'Breuer' adiabatic

$$\Delta_{\rm a}S^{\rm Br} \equiv -\beta_{\rm L}Q_{\rm L} - \beta_{\rm R}Q_{\rm R} - \Delta\left\langle\ln\rho^{\rm ss}_{\rm S}\right\rangle, \tag{2.70}$$

and the non-adiabatic one

$$\Delta_{\rm na} S^{\rm Br} = D[\rho_{\rm S}(0)||\rho_{\rm S}^{\rm ss}] - D[\rho_{\rm S}(t)||\rho_{\rm S}^{\rm ss}]. \tag{2.71}$$

Both terms are different from those of the 'Poised' case. Moreover here the non-adiabatic contribution (2.70) is positive only in the Markovian case. Their time derivatives are expressed respectively as:

$$\dot{S}_{\rm a}^{\rm Br} = -{\rm tr}\dot{\rho}_{\rm S}(t)\ln\rho_{\rm S}^{\rm ss} - {\rm tr}\dot{\rho}_{\rm L}(t)\ln\rho_{\rm L}^{\rm eq} - {\rm tr}\dot{\rho}_{\rm R}(t)\ln\rho_{\rm R}^{\rm eq}, \tag{2.72}$$

and

$$\dot{S}_{\rm na}^{\rm Br} = -{\rm tr}\dot{\rho}_{\rm S}(t)(\ln\rho_{\rm S}(t) - \ln\rho_{\rm S}^{\rm ss}). \tag{2.73}$$

In the late time limit one expects the adiabatic rate $\dot{S}_{\rm a}^{\rm Br}$ to be a positive quantity, since it has to coincide with the entropy production rate $\mathrm{d}\Delta_{\rm i}S/\mathrm{d}t$, instead the non-adiabatic rate $\dot{S}_{\rm na}^{\rm Br}$ clearly vanishes. It is not possible to establish their sign at generic time, unless the dynamics is Markovian, where in analogy with (2.14) $\dot{S}_{\rm na}^{\rm Br} \geq 0$.

Chapter 3

The model

The QBM Hamiltonian represents an harmonic oscillator bi-linearly coupled with coupling constants ϵ_i to a bath of N harmonic oscillators:

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{I}}; \tag{3.1}$$
$$H_{\mathrm{S}} = \frac{1}{2}\left(\omega_0^2 Q_0^2 + P_0^2\right) \quad , \quad H_{\mathrm{B}} = \frac{1}{2}\sum_{i=1}^{N}\left(\omega_i^2 Q_i^2 + P_i^2\right) \quad , \quad H_{\mathrm{I}} = \sum_{i=1}^{N}\epsilon_i Q_0 Q_i.$$

We have put all masses equal to one for simplicity.

The equations of motion in the Heisenberg picture read

$$\dot{Q}_\mu(t) = \frac{\mathrm{i}}{\hbar}\left[H, Q_\mu(t)\right] \quad , \quad \dot{P}_\mu(t) = \frac{\mathrm{i}}{\hbar}\left[H, P_\mu(t)\right]. \tag{3.2}$$

The Greek indices μ and ν include by convention also the central oscillator and the terms associated to the bath, while the Latin ones only run on the bath degrees of freedom. For convenience, we will use the shorthand notation $Q = Q_0$ and $P = P_0$. The solution of the equations of motion reads [Ullersma, 1966, Haake and Reibold, 1985]

$$Q_\mu(t) = \sum_{\mu=0}^{N}\left(\dot{A}_{\mu\nu}(t)Q_\nu(0) + A_{\mu\nu}(t)P_\nu(0)\right) \quad , \quad P_\mu(t) = \dot{Q}_\mu(t). \tag{3.3}$$

It is obtained by first finding a matrix transformation into new conjugate operators $\{Q'_\mu, P'_\mu\}$ which diagonalize the Hamiltonian into a set of $N+1$ normal harmonic oscillators, by then writing the Heisenberg solutions in that basis, and by finally transforming back to the original operators. The functions $A_{\mu\nu}(t)$ can be expressed in terms of the function

$$g(z) = z^2 - \omega_0^2 - \sum_{i=1}^{N}\frac{\epsilon_i^2}{z^2 - \omega_i^2}, \tag{3.4}$$

whose zeros z_ν, $\nu = 0, \ldots, N$, are the normal frequencies of the harmonic oscillators in the new basis. We have in fact

$$A_{\mu\nu}(t) = \sum_{\rho=0}^{N} X_{\mu\rho} X_{\nu\rho} \frac{\sin(z_\rho t)}{z_\rho}, \tag{3.5}$$

where the elements $X_{\mu\nu}$ of the transformation matrix are given by

$$X_{0\nu} = \left[\frac{1}{2z} \left. \frac{\mathrm{d}g(z)}{\mathrm{d}z} \right|_{z=z_\nu} \right]^{-1/2}, \qquad \nu = 0, \ldots, N; \tag{3.6}$$

$$X_{i\nu} = \frac{\epsilon_i}{z_\nu^2 - \omega_i^2} X_{0\nu}, \qquad i = 1, \ldots, N; \quad \nu = 0, \ldots, N. \tag{3.7}$$

From (3.4) one gets also a condition to be fulfilled in order to obtain a positive-definite Hamiltonian and non diverging solutions:

$$\Omega_0^2 = \omega_0^2 - \sum_{i=1}^{N} \frac{\epsilon_i^2}{\omega_i^2} \geq 0. \tag{3.8}$$

Ω_0 actually defines a normalized frequency of the central oscillator, as it emerges in the following Quantum Langevin Equation (QLE) (3.10). The role of the term $A(t) \equiv A_{00}$ is that of a retarded propagator (see [Fleming et al., 2011]). To see it, we first exploit the explicit solution to write down the equations of motion for the position operators in the bath as integro-differential equations involving the position operator of the central oscillator:

$$Q_i(t) = Q_i(0) \cos(\omega_i t) + \frac{P_i(0)}{\omega_i} \sin(\omega_i t) - \frac{\epsilon_i}{\omega_i} \int_0^t \mathrm{d}s \ \sin[\omega_i(t-s)] Q(s). \tag{3.9}$$

Then the central oscillator satisfies the following QLE which we express in a matrix representation:

$$\dot{\boldsymbol{z}}(t) + \boldsymbol{H} * \boldsymbol{z}(t) = -\boldsymbol{\eta}(t) - \boldsymbol{F}(t). \tag{3.10}$$

In this expression, $*$ represents the time convolution, $\boldsymbol{H}(t)$ is given by

$$\boldsymbol{H}(t) = \begin{bmatrix} 0 & -\delta(t) \\ \Omega_0^2 \delta(t) & K(t) \end{bmatrix}; \tag{3.11}$$

and we have defined $\boldsymbol{z}(t)$ with $\boldsymbol{z}^\mathsf{T}(t) = (Q(t), P(t))$ and the noise $\boldsymbol{\eta}^\mathsf{T}(t) = (0, \eta(t))$ with components

$$\eta(t) = \sum_i^N \epsilon_i \left[Q_i(0) \cos \omega_i t + \frac{P_i(0)}{\omega_i} \sin \omega_i t \right]. \tag{3.12}$$

The damping kernel $K(t)$ is defined by

$$K(t) = \int_0^\infty \mathrm{d}\omega \, \frac{\gamma(\omega)}{\omega^2} \cos \omega t, \tag{3.13}$$

where $\gamma(\omega)$ is the coupling strength

$$\gamma(\omega) = \sum_i \epsilon_i^2 \, \delta(\omega - \omega_i), \tag{3.14}$$

and $\mathbf{F}(t) = (0, K(t)Q(0))$ is the forcing term, which is responsible in the continuum limit for a fast slip of the initial conditions (see section 3.3).

The solution of the differential equation (3.10) can be easily obtained by taking the Laplace transform and then transforming back. One obtains

$$z(t) = \mathbf{\Phi}(t)z(0) - (\mathbf{\Phi} * \boldsymbol{\eta})(t). \tag{3.15}$$

Both terms contain the matrix propagator $\mathbf{\Phi}(t)$

$$\mathbf{\Phi}(t) = \begin{bmatrix} \dot{A}(t) & A(t) \\ \ddot{A}(t) & \dot{A}(t) \end{bmatrix}, \tag{3.16}$$

which depends on the damping kernel $K(t)$ via the propagator $A(t)$. The Laplace transform of $A(t)$ is given by

$$\widehat{A}(s) = \frac{1}{s^2 + s\widehat{K}(s) + \Omega_0^2}. \tag{3.17}$$

In A.1 we show that the Ullersma solution (3.3) and the Fleming one (3.9,3.15) are equivalent.

Having determined the time evolution of the Heisenberg momenta and positions as functions of the same operators at time $t = 0$, all the moments of these quantities at time t can now be evaluated as functions of the moments at $t = 0$ and of the $A_{\mu\nu}$'s.

3.1 Initial conditions

General initial conditions were specified in equation (2.2). An equivalent description of the system can be obtained via the Wigner quasi-probability distribution (often simply called "Wigner"), a function of the phase-space variables $(q, p) = (q_0, p_0, \ldots, q_N, p_N)$, defined in term of the total density matrix ρ by

$$W(q,p) = \frac{1}{(\pi\hbar)^N} \int_{-\infty}^{\infty} \prod_\mu \mathrm{d}y_\mu \, \mathrm{e}^{\mathrm{i}p_\mu y_\mu/\hbar} \left\langle q_0 - \frac{y_0}{2}, \ldots, q_N - \frac{y_N}{2} \middle| \rho \middle| q_0 + \frac{y_0}{2}, \ldots, q_N + \frac{y_N}{2} \right\rangle. \tag{3.18}$$

The reduced Wigner corresponding to the central oscillator and the bath reduced density matrix can be defined in a similar way and can be obtained from the total system Wigner by integrating out the appropriate degrees of freedom.

Using a matrix formalism with vectors $\tilde{z}^{\mathsf{T}} = (p, q)$, $z^{\mathsf{T}} = (Q, P)$ and $\boldsymbol{k}^{\mathsf{T}} = (k_q, k_p)$, a generic single-particle Gaussian Wigner and its Fourier transform read [Agarwal, 1971]:

$$W(q,p) = \frac{1}{\sqrt{2\pi\Delta^2}} \exp\{-\frac{(\tilde{\boldsymbol{z}} - \langle\tilde{\boldsymbol{z}}\rangle)^{\mathsf{T}}\boldsymbol{\sigma}(\tilde{\boldsymbol{z}} - \langle\tilde{\boldsymbol{z}}\rangle)}{2\Delta^2}\}; \tag{3.19}$$

$$\widetilde{W}(\boldsymbol{k}) = \exp\{-\frac{1}{2}\boldsymbol{k}^{\mathsf{T}}\boldsymbol{\sigma}\boldsymbol{k} - \mathrm{i}\boldsymbol{k}^{\mathsf{T}}\langle z\rangle\}. \tag{3.20}$$

The first moments and the symmetric covariance matrix respectively read $\langle\tilde{z}\rangle^{\mathsf{T}} = (\langle P\rangle, \langle Q\rangle)$, $\langle z\rangle^{\mathsf{T}} = (\langle Q\rangle, \langle P\rangle)$ and $\boldsymbol{\sigma}_{ij} = \left\langle\{z_i, z_j\}\right\rangle/2 - \langle z_i\rangle\left\langle z_j\right\rangle$ with $i, j = 1, 2$, where we denote by $\{\ldots,\ldots\}$ the anticommutator and by $\langle\ldots\rangle$ the average over a Gaussian density matrix ρ. We also define

$$\Delta = \left(\sigma_q^2\sigma_p^2 - C_{qp}^2\right)^{\frac{1}{2}} = (\det\boldsymbol{\sigma})^{\frac{1}{2}}, \tag{3.21}$$

where we indicate $\sigma_q^2 = \boldsymbol{\sigma}_{11}$, $\sigma_p^2 = \boldsymbol{\sigma}_{22}$ and $C_{qp} = \boldsymbol{\sigma}_{12}$.

We shall only consider initial conditions such that the Wigner of the central oscillator has a Gaussian expression at time $t = 0$. Then the Wigner is parametrized by its moments $\langle Q(0)\rangle$, $\langle P(0)\rangle$, $\left\langle Q^2(0)\right\rangle$, $\left\langle P^2(0)\right\rangle$ and $C_{pq}(0)$, given by $C_{qp}(0) = \langle\{Q(0) - \langle Q(0)\rangle, P(0) - \langle P(0)\rangle\}\rangle/2$. Since the initial density matrix of the bath is a product of exponentials of quadratic Hamiltonians, its corresponding Wigner is a product of Gaussian states which are parametrized, for $i = 1, \ldots, N$, by the moments

$$\begin{aligned} &\langle Q_i(0)\rangle = \langle P_i(0)\rangle = \langle\{Q_i(0), P_i(0)\}\rangle = 0, \\ &\left\langle Q_i^2(0)\right\rangle = \frac{E(\omega_i, T)}{\omega_i^2} \ , \ \left\langle P_i^2(0)\right\rangle = E(\omega_i, T), \end{aligned} \tag{3.22}$$

where

$$E(\omega, T) = \frac{\hbar\omega}{2}\coth\frac{\hbar\omega}{2T}. \tag{3.23}$$

As a result the initial total Wigner is also Gaussian.

3.2 Evolution

At time $t > 0$ the total density matrix operator will evolve in a unitary way (2.4) and the central oscillator and the bath will be correlated. The corresponding total

Wigner satisfies the Liouville-like evolution equation [Haake and Reibold, 1985, Zurek, 2003]

$$\frac{\partial}{\partial t}W(q,p,t) = [H,W]_{\rm PB}\,, \tag{3.24}$$

where H (3.1) is now considered as a function of the phase-space variables $(q,p) = (q_0,p_0,\ldots,q_N,p_N)$ and where $[\ldots,\ldots]_{\rm PB}$ are the Poisson brackets. Again, by the linearity of the dependence of the solution for (q,p) on the initial conditions, an initial Gaussian distribution remains Gaussian at later times. This means that the Wigner is a real Gaussian, positive definite at all times, and fully characterized by its first and second moments. This also applies to the bath and will be useful to evaluate its entropy as we are going to see in section 6.

It was shown in refs. [Haake and Reibold, 1985, Fleming et al., 2011] that the reduced Wigner satisfies the following partial differential equation:

$$\frac{\partial}{\partial t}W_{\rm S}(z,t) = \left[\nabla_z^{\mathsf{T}}\cdot\boldsymbol{\mathcal{H}}(t)\cdot z + \nabla_z^{\mathsf{T}}\cdot\boldsymbol{D}(t)\cdot\nabla_z\right]W_{\rm S}(z,t), \tag{3.25}$$

where the *pseudo-Hamiltonian* $\boldsymbol{\mathcal{H}}(t)$ and *diffusion* $\boldsymbol{D}(t)$ matrices are respectively given by

$$\boldsymbol{\mathcal{H}}(t) \equiv \begin{bmatrix} 0 & -1 \\ \Omega_{\rm R}^2(t) & 2\Gamma(t) \end{bmatrix} = -\dot{\boldsymbol{\Phi}}(t)\boldsymbol{\Phi}^{-1}(t), \tag{3.26}$$

$$\boldsymbol{D}(t) \equiv \begin{bmatrix} 0 & -\frac{1}{2}D_{qp}(t) \\ -\frac{1}{2}D_{qp}(t) & D_{pp}(t) \end{bmatrix} = \frac{1}{2}\left[\boldsymbol{\mathcal{H}}(t)\boldsymbol{\sigma}_T(t) + \boldsymbol{\sigma}_T(t)\boldsymbol{\mathcal{H}}^{\mathsf{T}}(t) + \dot{\boldsymbol{\sigma}}_T(t)\right], \tag{3.27}$$

where $\boldsymbol{\Phi}(t)$ is the matrix propagator (3.16) and the thermal covariance matrix $\boldsymbol{\sigma}_T(t)$ is defined by

$$\boldsymbol{\sigma}_T(t) = \begin{bmatrix} \sigma_{q,T}^2 & C_{qp,T} \\ C_{qp,T} & \sigma_{p,T}^2 \end{bmatrix} = \int_0^t {\rm d}\tau \int_0^t {\rm d}\tau'\ \boldsymbol{\Phi}(t-\tau)\begin{bmatrix} 0 & 0 \\ 0 & \nu(\tau-\tau') \end{bmatrix}\boldsymbol{\Phi}^{\mathsf{T}}(t-\tau'). \tag{3.28}$$

The noise kernel is defined as

$$\nu(t) = \frac{1}{2}\langle\{\eta(t),\eta(0)\}\rangle = \int_0^\infty {\rm d}\omega\ \frac{\gamma(\omega)}{\omega^2}\,E(\omega,T)\,\cos\omega t, \tag{3.29}$$

so that we have explicitly

$$\boldsymbol{\sigma}_T(t) = \int_0^\infty {\rm d}\omega\ \frac{\gamma(\omega)}{\omega^2}\,E(\omega,T)\begin{bmatrix} \left|\int_0^t {\rm d}t'\ A(t'){\rm e}^{i\omega t'}\right|^2 & \frac{1}{2}\frac{\rm d}{{\rm d}t}\left|\int_0^t {\rm d}t'\ A(t'){\rm e}^{{\rm i}\omega t'}\right|^2 \\ \frac{1}{2}\frac{\rm d}{{\rm d}t}\left|\int_0^t dt' A(t'){\rm e}^{{\rm i}\omega t'}\right|^2 & \left|\int_0^t {\rm d}t'\ \dot{A}(t'){\rm e}^{{\rm i}\omega t'}\right|^2 \end{bmatrix}. \tag{3.30}$$

$\boldsymbol{\mathcal{H}}(t)$ and $\boldsymbol{D}(t)$ depend on the coupling strength via the damping and noise kernels. The off-diagonal elements of the diffusion matrix are called the *anomalous diffusion coefficients*.

The solution of equation (3.25) can be found by a Fourier transformation, via the method of characteristics [Fleming et al., 2011]:

$$\widetilde{W}_{\mathrm{S}}(\boldsymbol{k},t) = \widetilde{W}_{\mathrm{S}}(\boldsymbol{\Phi}^{\mathsf{T}}(t)\boldsymbol{k},0)\,\mathrm{e}^{-\frac{1}{2}\boldsymbol{k}^{\mathsf{T}}\boldsymbol{\sigma}_T(t)\boldsymbol{k}}, \tag{3.31}$$

which appears as a product of a function depending on the Wigner at time zero $\widetilde{W}_{\mathrm{S}}(\boldsymbol{k},0)$, times a Gaussian one containing the thermal covariance. It clearly assumes Gaussian form in our hypotheses where the initial $\tilde{W}_S(\boldsymbol{k},0)$ is Gaussian (3.20). The dynamics of the central oscillator is then fully described by the first and second moments of the position and momentum operators:

$$\langle z(t)\rangle = \boldsymbol{\Phi}(t)z_0; \tag{3.32}$$

$$\boldsymbol{\sigma}(t) = \boldsymbol{\Phi}(t)\boldsymbol{\sigma}_0\boldsymbol{\Phi}^{\mathsf{T}}(t) + \boldsymbol{\sigma}_T(t). \tag{3.33}$$

The general covariance matrix $\boldsymbol{\sigma}(t)$ corresponds to the covariance matrix in (3.19) if the averages $\langle\ldots\rangle$ are evaluated with the total density operator at time t (2.4). It appears as the sum of the contribution of the evolution of the initial conditions and of the thermal covariance. The same expressions can be found by taking the average over initial conditions of the operators in the Heisenberg form (3.3), expressing the $A_{i0}(t)$'s as functions of $A(t)$ (A.1) and by then using the coupling strength (3.14) [Haake and Reibold, 1985]. The elements of the correlation matrix are reported in more detail in A.2.

At finite sizes one expects oscillatory behavior both for the dissipation and the diffusion coefficients. As in Ref. [Ullersma, 1966], in the following we are going to assume an Ohmic form with a large cut-off for the couplings ϵ_i^2 in (3.14). This choice enables us to obtain time-independent dissipation coefficients in the continuum frequency limit, while the diffusion ones only become time-independent in certain limits such as the high temperature limit. In general, however, this would not be the case: by assuming for example a sub-Ohmic coupling with a slower decay for larger frequencies, one would have time-dependent and nonlocal dissipation and diffusion coefficients at all times, even in the high-temperature limit [Fleming et al., 2011].

3.3 Thermodynamic limit

The thermodynamic limit of an infinite number of bath oscillators is obtained by substituting a continuous function $\gamma(\omega)$ to the discrete coupling strength (3.14). We choose the Drude-like Ullersma coupling strength [Haake and Reibold, 1985, Ullersma, 1966]

$$\gamma(\omega) = \frac{2}{\pi}\frac{\kappa\alpha^2\omega^2}{\alpha^2+\omega^2}. \tag{3.34}$$

The parameter κ tunes the strength of the coupling, while the cut-off α, which is introduced in order to eliminate ultra-violet divergences, can be associated to the bath memory time. In fact the damping kernel (3.13) with this coupling strength is given by

$$K(t) = \kappa\alpha\, \mathrm{e}^{-\alpha t}, \tag{3.35}$$

and thus decays over times of order α^{-1}.

The general form of the propagator $A(t)$ following from the strength (3.34) can be found in [Haake and Reibold, 1985]. It is characterized by three time scales: Ω, Γ and λ, deriving from the poles λ, $\Gamma \pm i\Omega$ of the Laplace transform of the propagator (3.17). They are obtained by solving the following equations in which the bare central oscillator frequency ω_0, the coupling κ and the cut-off α appear:

$$\lambda + 2\Gamma = \alpha \ , \ \Omega^2 + \Gamma^2 + 2\Gamma\lambda = \omega_0^2 \ , \ \left(\Omega^2 + \Gamma^2\right)\frac{\lambda}{\alpha} = \omega_0^2 - \kappa\alpha. \tag{3.36}$$

In this situation, the renormalized frequency Ω_0 (3.8) of the central oscillator is simply given by

$$\Omega_0^2 = \omega_0^2 - \kappa\alpha. \tag{3.37}$$

The propagator $A(t)$ describes a noisy damped oscillator, where Ω is the characteristic frequency and λ and Γ characterize the damping rates. When the time scale $1/\lambda$ is much shorter than $1/\Gamma$ and $1/\Omega$, the damping kernel $K(t)$ (3.13) becomes delta-like and the evolution equation (3.10) becomes local in time. This is obtained by taking the large cut-off limit, defined by

$$\alpha \gg \kappa, \omega_0. \tag{3.38}$$

We can then approximate (3.36) by

$$\lambda \simeq \alpha \ , \ \Gamma \simeq \kappa/2 \ , \ \Omega_0^2 \simeq \Gamma^2 + \Omega^2, \tag{3.39}$$

and the propagator $A(t)$ assumes the form

$$A_{\mathrm{loc}}(t) = \frac{1}{\Omega}\sin(\Omega t)\mathrm{e}^{-\Gamma t}, \tag{3.40}$$

which is typical of a damped Ornstein-Uhlenbeck process. One can observe in fact that the pseudo-Hamiltonian $\boldsymbol{\mathcal{H}}(t)$, at $\mathrm{O}\,(1/\alpha)$ and for $t \gg 1/\alpha$, becomes equal to the the time-independent matrix

$$\boldsymbol{\mathcal{H}}_{\mathrm{loc}} = \begin{bmatrix} 0 & -1 \\ \Omega_0^2 & 2\Gamma \end{bmatrix}. \tag{3.41}$$

Since Ω_0 is real, the transition between real and imaginary Ω corresponds to the transition between the under-damped ($\Gamma < \Omega_0$) and the over-damped regimes ($\Gamma >$

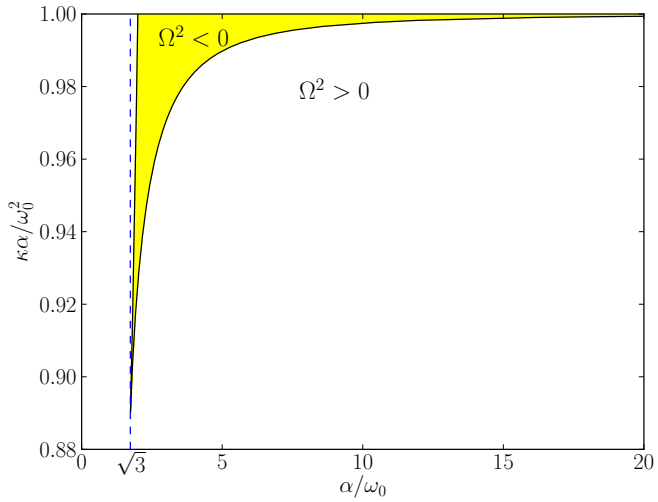

Figure 3.1: Transition between real (white) and imaginary (yellow) Ω. In the large cut-off limit (3.38) it corresponds to the transition between under-damping $\Gamma < \Omega_0$ and over-damping $\Gamma > \Omega_0$. For $\alpha/\omega_0 \leq \sqrt{3}$ (on the left of the dotted line) one always has $\Omega^2 > 0$.

Ω_0). The quantum and time-dependence features of our process are then contained only in the noise kernel (3.29),

$$\nu(t) = -\kappa\alpha^2 \left(\frac{1}{2} \cot \frac{\beta\alpha}{2} \mathrm{e}^{-\alpha t} + \frac{1}{\pi} \sum_{\ell=1}^{\infty} \frac{\ell}{(\alpha\tau_\beta)^2 - \ell^2} \mathrm{e}^{-\ell t/\tau_\beta} \right), \tag{3.42}$$

where we have defined

$$\tau_\beta = \frac{\hbar\beta}{2\pi}. \tag{3.43}$$

We can thus define the following limits:

The low-temperature limit:

$$\alpha \gg 1/\tau_\beta; \tag{3.44}$$

The high-temperature classical limit:

$$1/\tau_\beta \gg \alpha; \tag{3.45}$$

The weak-coupling limit:

$$\Gamma \ll \Omega, 1/\tau_\beta. \tag{3.46}$$

The noise kernel determines the thermal covariance matrix $\boldsymbol{\sigma}_\beta$ (3.28) and, via (3.27), the diffusion coefficients of the ME. Thus the quantum and time-dependence features will show up in these quantities. One can evaluate the covariance matrix by using the local propagator (3.40) inside the general expression (3.30), up to terms of $\mathrm{O}(1/\alpha)$. Using this propagator instead of the general one (see [Haake and Reibold, 1985, eq.(7.10)]) does not affect either the covariance thermal matrix or the diffusion coefficients in the large cut-off limit, even for times $t < 1/\alpha$, since only correction of $\mathrm{O}(1/\alpha)$ arise [Fleming et al., 2011]. Since the coupling strength (3.34) is an even meromorphic function, the integrals appearing in (3.30) can be evaluated by a contour integration in the complex plane.

Complete expression for the thermal correlation matrix in the large cut-off limit, which are exploited in the following for the calculation of the entropies, were derived in [Haake and Reibold, 1985] and are reported in A.2. Their quantum features are due to the presence of the function $E(\omega, T)$, whose poles at $\omega = \mathrm{i}k\,2\pi/\tau_\beta$ with k any integer, give rise to the thermal transients, i.e., to terms which vanish on a time scale of order τ_β. These terms are also responsible for the time-dependence of the diffusion coefficients of the master equation [Haake and Reibold, 1985]. In the high-temperature classical limit, where $E(\omega, T)$ approaches T, all the thermal transients vanish and the expressions of the covariance matrix simplify.

One can deduce from equations (3.16), (3.31) and (3.40) that, since $\lim_{t\to\infty} A_{\mathrm{loc}}(t) = 0$, in the thermodynamic limit the system eventually loses all information on its initial conditions, and its distribution assumes the characteristic Gaussian form corresponding to the late-time thermal covariance matrix, as described in the next subsection.

An important feature of this model is the presence of initial slips in the momentum average, in the non-thermal part of the averaged square momentum and of the correlation between Q and P. Using the local propagator (3.40) from $t = 0$, implies neglecting an initial evolution of the system during a short time of order $1/\alpha$, in which the central oscillator is subjected to an initial kick [Fleming et al., 2011, Haake and Reibold, 1985]. One can easily observe, indeed, that

$$\ddot{A}(0) = 0 \neq \ddot{A}_{\mathrm{loc}}(t{=}0^+) = -2\Gamma. \tag{3.47}$$

Our description will thus only be valid for $t \gg 1/\alpha$. The effect of initial slips both on the moments and on the definitions of entropy production is discussed in A.3.

Late-time covariance matrix

In the thermodynamical limit it is possible to evaluate the long-time behavior of the diffusion coefficients and of the covariance thermal matrix. They are related

by

$$D_{qp}(\infty) = \left\langle P^2(\infty) \right\rangle - \Omega_0^2 \left\langle Q^2(\infty) \right\rangle ; \tag{3.48}$$

$$D_{pp}(\infty) = 2\Gamma \left\langle P^2(\infty) \right\rangle . \tag{3.49}$$

Thus the anomalous diffusion coefficients survive, since the right-hand side of the first equation of (3.48) does not vanish. This implies that equipartition does not hold in the general quantum case.

Interestingly, as observed in [Haake and Reibold, 1985], one obtains

$$\left\langle Q^2(\infty) \right\rangle = \left\langle Q^2 \right\rangle_{\rm eq} \ , \ \left\langle P^2(\infty) \right\rangle = \left\langle P^2 \right\rangle_{\rm eq} , \tag{3.50}$$

namely that the stationary form of the central oscillator density matrix at $t = \infty$ equals the traced canonical equilibrium one of the total system:

$$\rho_{\rm S}(\infty) = \rho_{\rm S}^{\rm st} = {\rm tr}_{\rm B}\rho^{\rm eq} \ , \ \rho^{\rm eq} \equiv \frac{{\rm e}^{-\beta H}}{Z} \ , \ Z = {\rm tr}{\rm e}^{-\beta H}. \tag{3.51}$$

This does not mean of course that the total system equilibrates: $\rho(\infty) \neq \rho^{\rm eq}$ [Hilt et al., 2011]. Furthermore, it has been shown in [Grabert et al., 1984] that

$$\rho_{\rm S}(\infty) = \rho_{\rm S}^{\rm eq} \equiv \frac{{\rm e}^{-\beta H_{\rm S}^{\rm eq}}}{Z_{\rm S}^{\rm eq}} \ , \ Z_{\rm S}^{\rm eq} = {\rm tr}_{\rm S}{\rm e}^{-\beta H_{\rm S}^{\rm eq}}, \tag{3.52}$$

where the equilibrium effective Hamiltonian $H_{\rm S}^{\rm eq}$ is given by

$$H_{\rm S}^{\rm eq} = \frac{1}{2M_{\rm eff}}P^2 + \frac{1}{2}M_{\rm eff}\omega_{\rm eff}^2 Q^2. \tag{3.53}$$

The effective frequency $\omega_{\rm eff}$ and mass $M_{\rm eff}$ are respectively given by

$$\omega_{\rm eff} = \frac{2}{\beta\hbar}\coth^{-1}\left(\frac{2}{\hbar}\sqrt{\langle Q^2\rangle_{\rm eq}\langle P^2\rangle_{\rm eq}}\right) \ , \ M_{\rm eff} = \frac{1}{\omega_{\rm eff}}\sqrt{\frac{\langle P^2\rangle_{\rm eq}}{\langle Q^2\rangle_{\rm eq}}}. \tag{3.54}$$

Expressions for $\left\langle Q^2 \right\rangle_{\rm eq}$ and $\left\langle P^2 \right\rangle_{\rm eq}$ can be found in [Grabert et al., 1984] and [Haake and Reibold, 1985], and are reported in (A.19,A.20).

It is worth noticing that the traced canonical equilibrium density matrix (3.52) can be equivalently written in the form [Hänggi et al., 2008, Hänggi and Ludwig Ingold, 2006]:

$$\rho_{\rm S}^{\rm eq} = \frac{{\rm e}^{-\beta H_{\rm S}^{\rm MF}}}{Z_{\rm S}^{\rm MF}} \ , \ H_{\rm S}^{\rm MF} = -\frac{1}{\beta}\ln\frac{{\rm tr}e^{-\beta H}}{Z_{\rm B}} \ , \ Z_{\rm S}^{\rm MF} = \frac{Z}{Z_{\rm B}} \ , \tag{3.55}$$

where an Hamiltonian of mean force H_S^{MF} has been introduced, which differs from the effective H_S^{eq} by the additive constant $-\beta(\ln Z_S^{MF} - \ln Z_S^{eq})$. Both partition functions have a well-known analytical expression [Grabert et al., 1984]. For the practical purpose of evaluating the Breuer entropy flow (2.16) we will use the effective Hamiltonian. However we emphasize that the use of the mean force Hamiltonian leads to exactly the same entropy production (since only the density matrix is involved) and heat flow (since only differences in energies are considered).

The identities (3.50,3.51,3.52) do not generally hold in open quantum systems. They are however an important feature of our bilinear model and hold independently of the choice of the continuous limit strength.

Chapter 4

Explicit forms of the entropy production

We report here the explicit forms of the entropy production, according to the P (2.9), the ELB (2.17) and the 'Breuer' expression obtained in (2.13). To evaluate them one needs to know the expressions of the entropy and the entropy flow.

Since the central oscillator density matrix is Gaussian at each time t, its von Neumann entropy entropy is given by [Agarwal, 1971]

$$\begin{aligned} S(t) &= -\mathrm{tr}_{\mathrm{S}}\rho_{\mathrm{S}}(t)\ln\rho_{\mathrm{S}}(t) \\ &= \left(\Delta(t)+\frac{1}{2}\right)\ln\left(\Delta(t)+\frac{1}{2}\right)-\left(\Delta(t)-\frac{1}{2}\right)\ln\left(\Delta(t)-\frac{1}{2}\right), \end{aligned} \tag{4.1}$$

where we have defined

$$\Delta(t)=\hbar^{-1}\left(\sigma_q^2(t)\sigma_p^2(t)-C_{qp}^2(t)\right)^{1/2}, \tag{4.2}$$

which is a function of the correlation matrix at time t. One notices that $S(t)$ is well defined if the uncertainty principle is satisfied.

The 'Poised' entropy production can be written as

$$\Delta_{\mathrm{i}}S^{\mathrm{P}}=\Delta S-\Delta_{\mathrm{e}}S^{\mathrm{P}}; \tag{4.3}$$

$$\Delta_{\mathrm{e}}S^{\mathrm{P}}=\mathrm{tr}\left(\rho_S(0)-\rho_S(t)\right)\ln\rho_S^*(t). \tag{4.4}$$

The 'Poised' density matrix $\rho_S^*(t)$ is Gaussian with vanishing means of Q and P (as shown in A.4) and is given by

$$\ln\rho_S^*(t)=-\frac{1}{2}\ln\left(\Delta^{*2}(t)-\frac{1}{4}\right)-\frac{\Lambda^*(t)}{2\hbar^2\Delta^*(t)}\ln\frac{\Delta^*(t)+\frac{1}{2}}{\Delta^*(t)-\frac{1}{2}}, \tag{4.5}$$

where we have defined

$$\Delta^*(t) = \hbar^{-1}\left(\sigma_q^{*2}(t)\sigma_p^{*2}(t) - {C_{qp}^*}^2(t)\right)^{1/2}; \tag{4.6}$$

$$\Lambda^*(t) = \sigma_p^{*2}(t)Q^2 + \sigma_q^{*2}(t)P^2 - C_{qp}^*(t)\{Q,P\}. \tag{4.7}$$

The variances and correlation ${\sigma_{q,p}^*}^2(t)$ and $C_{qp}^*(t)$ are given in A.4. Then one obtains

$$\Delta_{\mathrm{e}}S^{\mathrm{P}} = \frac{\langle\Lambda^*(t)\rangle_t - \langle\Lambda^*(t)\rangle_0}{2\hbar^2\Delta^*(t)}\ln\frac{\Delta^*(t)+\frac{1}{2}}{\Delta^*(t)-\frac{1}{2}}, \tag{4.8}$$

where we have defined, for any operator O acting on the Hilbert space of S, $\langle O\rangle_t = \mathrm{tr}\rho_{\mathrm{S}}(t)O$.

As for the Breuer entropy flow, $\Delta_{\mathrm{e}}S^{\mathrm{Br}}$ is straightforwardly given by the change in the effective energy $H_{\mathrm{S}}^{\mathrm{eq}}$ (3.53). Then one only needs to know position and momentum second moments at time t, which in the finite case are obtained from the first moments and from the correlation matrix which appear in (A.5)-(A.10), while in the continuum case one exploits the general expressions (3.32)-(3.30) with the Ullersma coupling strength (3.34) (see (A.12) and (A.13)). The entropy flow $\Delta_{\mathrm{e}}S$ is instead proportional to the change in the bath energy (2.20). To evaluate it, one needs rather to evaluate the average of the interaction energy term $\langle H_{\mathrm{I}}\rangle$. By using the Ullersma strength (3.34) in the large cut-off limit, it turns out that for $t \gg 1/\alpha$

$$\langle H_I(t)\rangle = D_{qp}(t) - \kappa\alpha\left\langle Q^2(t)\right\rangle, \tag{4.9}$$

where $D_{qp}(t)$ is the anomalous diffusion coefficient (3.27). This evaluation is reported in A.6. Thus, by comparing definitions (2.20) and (2.16), we obtain the difference between the two entropy flows is given by

$$\Delta S_{\,e} - \Delta_{\mathrm{e}}S^{\mathrm{Br}} = \beta\left[\Delta\langle H_{\mathrm{S}}\rangle - \Delta\left\langle H_{\mathrm{S}}^{\mathrm{eq}}\right\rangle - \kappa\alpha\left\langle Q^2(t)\right\rangle + D_{qp}(t)\right]. \tag{4.10}$$

The difference of entropy production is the same with opposite sign.

As already mentioned, the expressions we use in the continuum limit for the three definitions of entropy only apply for $t \gg 1/\alpha$, after the initial slip has taken place. Their contribution to entropy, which is reported in A.3, implies that the entropy flows and productions often do not start from 0, as one can observe in the following figures.

4.1 The Markovian case

Generally, in the limit of short-lived thermal transients, namely $\Gamma\tau_\beta \ll 1$, the generator of the dynamics $\mathcal{L}$ can be considered time-independent, since the diffusion

coefficients (3.27) are close to their $t = \infty$ limit (3.48). As we have seen in section 2.1, in this case the entropy production definition (2.13) and its time derivative turn out to be consistently positive, as the system equilibrium density matrix ρ_S^{eq} does not depend on time, and the entropy flow is given by the average variation of the effective system Hamiltonian H_S^{eq}, as already observed in equation (2.16). This holds both in the high-temperature classical and weak-coupling limits [Haake and Reibold, 1985].

4.1.1 Classical limit.

In the high-temperature classical limit (3.45) all the quantum features of the system disappear and the anomalous diffusion coefficient vanishes, thus recovering equipartition (3.48), since $\left\langle P^2 \right\rangle_{eq} = T$, and $\left\langle Q^2 \right\rangle_{eq} = T/\Omega_0^2$. In particular the equation satisfied by the Wigner has exactly the form of the Kramers equation for an oscillator in contact with a bath at temperature T [Kramers, 1940, Risken, 1989]. In this limit, since we have $\Delta(t) \gg 1$, $\forall t$, the system entropy (4.1) assumes its classical form for a Gaussian distribution

$$S(t) \simeq 1 + \ln \Delta(t), \tag{4.11}$$

Moreover the effective equilibrium energy is given by

$$H_S^{eq} \simeq \frac{1}{2}(\Omega_0^2 Q^2 + P^2). \tag{4.12}$$

Thus the definition (2.16) of the entropy flow reduces to that of stochastic thermodynamics, which is defined as the average variation of the effective energy of the system, namely the classical one with the renormalized frequency Ω_0 in place of ω_0. This means that the corresponding definition of the entropy production coincides in this limit with the one introduced in the theory of stochastic thermodynamics for the Kramers equation [Imparato and Peliti, 2006]. In the overdamped limit $\Gamma \gg \Omega_0$ the momentum equilibrates much faster than position and can thus be traced out. The entropy production assumes in this case the form proposed in the theory of stochastic thermodynamics for the overdamped Fokker-Planck equation [Seifert, 2005]. As long as momentum has not yet fully equilibrated, the latter expression constitutes a lower bound to the former one since it results from a coarse graining procedure (see, e.g., [Gomez-Marin et al., 2008]). Let us also note that by taking the weak coupling limit $\kappa \to 0$ one gets in (4.12) the bare frequency ω_0, and that then the entropy flow becomes exactly equal to the change in the central oscillator energy, divided by the temperature of the bath.

We show in Figure 4.1 the high-temperature limit (3.45) of the difference between the different definitions of the entropy production with different coupling

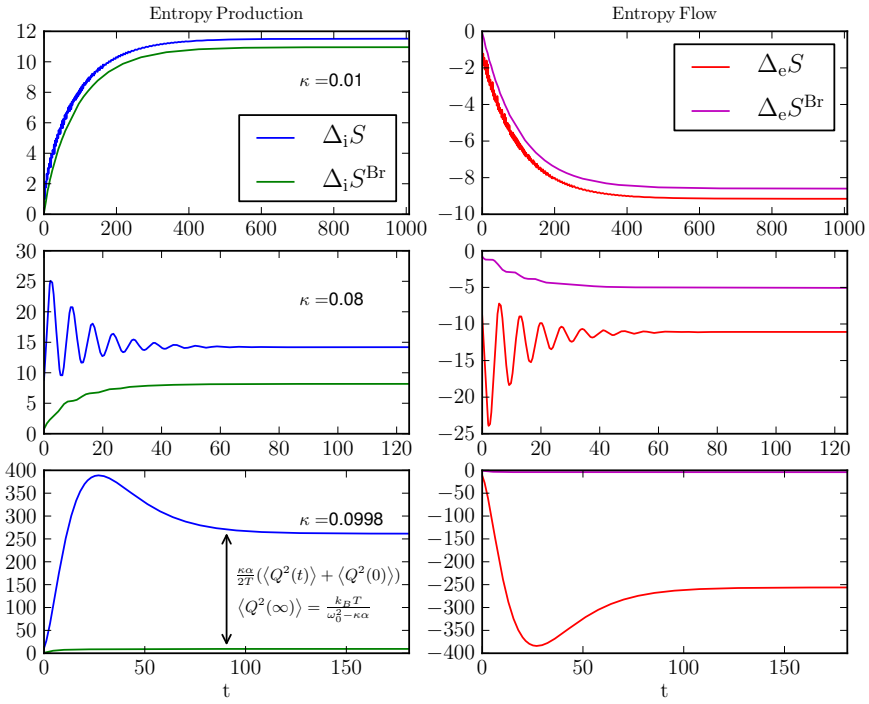

Figure 4.1: The different expressions for the entropy production (left) and the entropy flow (right), for different couplings κ (top and center underdamped, bottom overdamped) in the classical regime. The parameters are: temperature $T = 1000$, $\alpha = 10$, $\omega_0 = 1$, $\sigma_q^2(0) = 100$, $\sigma_p^2(0) = 100$, $C_{qp}(0) = 10$, $\langle Q(0)\rangle = 100$, $\langle P(0)\rangle = 100$.

strengths. In the classical limit the anomalous diffusion term in (4.9) vanishes and the normal diffusion coefficient is time independent. This means that the Poised and Breuer expressions for entropy become equal: $\Delta_i S^{\mathrm{Br}} = \Delta_i S^{\mathrm{P}}$. Considering also the expression assumed by H_S^{eq} (4.12), the expression (4.10) for the difference of flows simplifies to

$$\Delta_e S - \Delta_e S^{\mathrm{Br}} = -\frac{\beta}{2}\kappa\alpha\left(\left\langle Q^2(t)\right\rangle + \left\langle Q^2(0)\right\rangle\right). \tag{4.13}$$

The same difference with opposite sign holds for the entropy production. In the classical limit the thermal part of $\left\langle Q^2(t)\right\rangle$ is proportional to $1/\beta\Omega_0^2$. This means that the difference between the two expressions for the entropy production *diverges*, since for large κ one has

$$\Omega_0^2 = \omega_0^2 - \kappa\alpha \to 0. \tag{4.14}$$

This appears clearly in the figure, where the different expressions for the en-

tropy production $\Delta_{\mathrm{i}}S$ and for the entropy flow $\Delta_{\mathrm{e}}S$ are shown for different coupling strengths κ, both in the underdamped and the overdamped regime.

The difference between the definitions is due to the fact that the expression $\Delta_{\mathrm{i}}S$ and the corresponding expression $\Delta_{\mathrm{e}}S$ of the entropy flow both diverge in the limit (4.14) as $1/\Omega_0^2$,

$$\Delta_{\mathrm{e}}S(\infty) = 1 - \frac{1}{2}\frac{\kappa\alpha}{\Omega_0^2} - \frac{\beta}{2}\left(\omega_0^2\left\langle Q^2(0)\right\rangle + \left\langle P^2(0)\right\rangle\right). \tag{4.15}$$

However, the expression $\Delta_{\mathrm{i}}S^{\mathrm{Br}}$ diverges only logarithmically like the von Neumann entropy:

$$\Delta S(\infty) \simeq |\ln\beta\Omega_0| - S(0) \tag{4.16}$$

In fact the expression $\Delta_{\mathrm{e}}S^{\mathrm{Br}}$ does not diverge, since in the effective Hamiltonian (4.12) only the renormalized frequency appears: $M_{\mathrm{eff}}\omega_{\mathrm{eff}}^2 \to \Omega_0^2$.

One notices in Figure 4.1 that both expressions of the entropy productions are positive, but that the ELB one, $\Delta_{\mathrm{i}}S$, exhibits damped oscillations yielding a nonpositive time derivative. This can be directly seen from the fact that the time derivative of $\Delta_{\mathrm{i}}S^{\mathrm{Br}}$ is positive, due to the fact that the process is time independent (cf. sec. 4.1), and that the ELB one differs from it by a constant plus a term proportional to $\left\langle Q^2(t)\right\rangle$, which is characterized by damped oscillations.

We remark here that usually in literature the total Hamiltonian is renormalized by a self interaction term, such that no positivity condition similar to equation (3.8) has to be satisfied. In this case there would not be any divergence of $\left\langle Q^2(t)\right\rangle$, which would be proportional to T/ω_0^2, but the difference between the two definitions of the entropy production can be made arbitrarily large by taking $\kappa \to \infty$ [Nieuwenhuizen and Allahverdyan, 2002].

4.1.2 Weak-coupling limit

Another case in which the entropy flow is the equal to the one defined in stochastic thermodynamics is the weak-coupling limit in the general quantum setting $\Gamma \ll \Omega, \tau_\beta^{-1}$. Some care is needed, since the anomalous diffusion coefficient $D_{qp}(t)$ does not vanish at long times to first order in the coupling Γ, just as the normal diffusion coefficient $D_{pp}(t)$:

$$D_{qp}(\infty) = \frac{2}{\pi}\hbar\Gamma\,\mathrm{Re}\left[\psi(1+\lambda\tau_\beta) - \psi(1+i\Omega\tau_\beta)\right] + \mathrm{O}\left(\Gamma^2\right); \tag{4.17}$$

$$D_{pp}(\infty) = 2\Gamma E(\Omega, T) + \mathrm{O}\left(\Gamma^2\right), \tag{4.18}$$

where $\psi(z)$ is the digamma function. Anyway their contribution to $\left\langle Q^2\right\rangle_{\mathrm{eq}}$ is different as $D_{pp}(t)$ contributes to order one, while $D_{qp}(t)$ to order Γ as seen by inverting

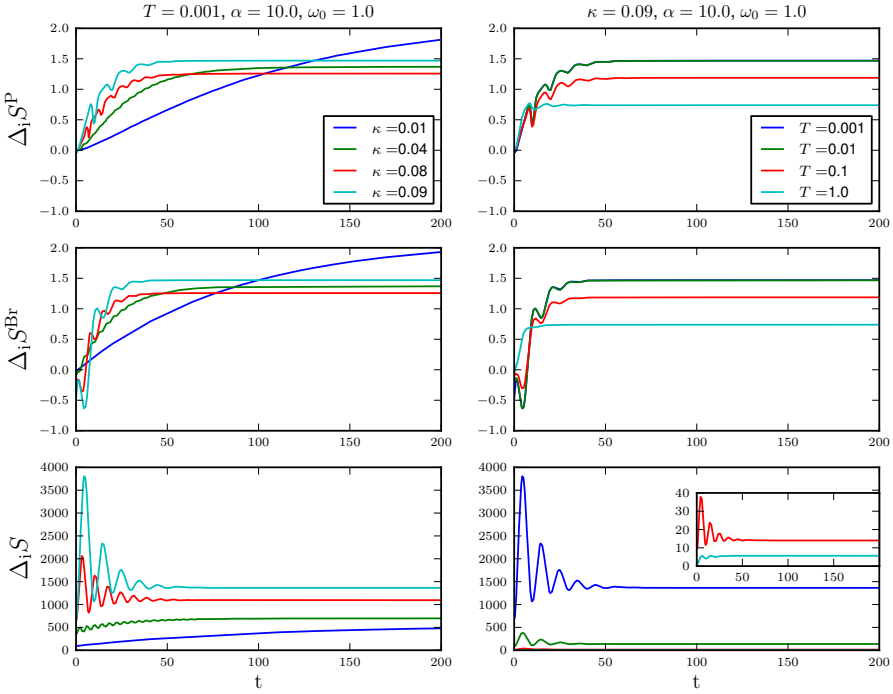

Figure 4.2: Entropy productions $\Delta_i S^P$, $\Delta_i S^{Br}$ and $\Delta_i S$ at different values of the coupling κ: 0.01 (blue), 0.04 (green), 0.08 (red), 0.09 (cyan) with temperature $T = 0.001$ (left), and different temperatures T: 0.001 (blue), 0.01 (green), 0.1 (red), 1.0 (cyan), with $\kappa = 0.09$ (right). Initial condition are fixed: $\sigma_q^2(0) = 1.0$, $\sigma_p^2(0) = 1.0$, $C_{qp}(0) = 0$, $\langle Q(0)\rangle = 0$, $\langle P(0)\rangle = 0$.

(3.48). One gets then equipartition to first order in Γ:

$$\left\langle Q^2 \right\rangle_{\text{eq}} = E(\Omega, T)/\Omega^2 + \mathrm{O}(\Gamma) \quad , \quad \left\langle P^2 \right\rangle_{\text{eq}} = E(\Omega, T) + \mathrm{O}(\Gamma), \tag{4.19}$$

where Ω can be approximated by Ω_0 to first order in Γ. This correspond to an equilibrium density matrix ρ_S^{eq} (3.52) corresponding to the equilibrium Hamiltonian

$$H_S^{\text{eq}} = \frac{1}{2}(\omega_0 Q^2 + P^2) \tag{4.20}$$

which is the same as the central oscillator one (3.1).

4.2 Low-temperature limit

In the low-temperature limit (3.44) one expects that the Breuer entropy production expression (2.13), as well as its time derivative, can become negative. The Poised and ELB expressions (2.17) remain instead positive, while their time derivative can be negative. As we observe in Figure 4.2, for sufficiently low temperature and strong couplings, the expression $\Delta_{\mathrm{i}} S^{\mathrm{Br}}$ becomes negative, exhibiting an oscillatory behavior. At higher temperatures or weaker couplings the amplitude of the oscillations becomes smaller. Thus in these limits one obtains a positive definite entropy production, as well as a positive time derivative. We observe that the Poised and Breuer entropy production have the same asymptotic value, as expected, since $\rho_{\mathrm{S}}^{*}(\infty) = \rho_{\mathrm{S}}^{eq}$.

One notices that also in the low-temperature limit (3.44) the ELB expression can be orders of magnitude larger than the other two, due to the coupling term $\kappa\alpha \left\langle Q^2(t) \right\rangle$ which appears in the entropy flow. This difference can be much larger respect to the classical case, due to the presence of the quantum terms contained in $\left\langle Q^2(t) \right\rangle$, which actually become more relevant than the classical one.

Chapter 5

Poincaré recurrences

When the number N of bath oscillators is finite, the dynamics is characterized by a recurrent behavior, with a period identified by the Poincaré recurrence time $t_{\mathrm{P}} \sim 2\pi/\min(z_{\nu+1} - z_\nu)$ [Ullersma, 1966], where the z_ν's are the normal frequencies. We can interpret this recurrence as an almost periodic return to the initial decoupled state. Interestingly, while $\Delta_{\mathrm{i}} S$ remains positive by definition, one might have a negative $\Delta_{\mathrm{i}} S^{\mathrm{Br}}$, even in the classical case. When the size of the bath becomes larger, the recurrence time grows, and one expects that the entropy approaches its typical irreversible behavior, eventually relaxing to the equilibrium asymptotic value.

In the present section we study this behavior in the two specific cases of uniform and Lorentzian frequency sampling, always assuming that the coupling strength converges to the Ullersma expression (3.34). Indeed, the density of states $\sum_i \delta(\omega - \omega_i)$ inside the coupling strength can be arbitrarily chosen. We evaluate the thermal covariance matrix components $\sigma^2_{q,T}(t)$, $\sigma^2_{p,T}(t)$, and the equilibrium symmetrized autocorrelation function $C(t)$, defined by

$$C(t) = \frac{1}{2} \langle \{Q(t), Q(0)\} \rangle_{\mathrm{eq}} \,. \tag{5.1}$$

We can also consider the Fourier transform of the correlation function $C(t)$. Indeed, in the classical limit, the finite-size correlation function has the expression

$$C_N(t) = T \sum_{\nu=0}^{N} \frac{X^2_{0\nu}}{z^2_\nu} \cos(z_\nu t). \tag{5.2}$$

We can thus represent the Fourier transform $\tilde{C}_N(\omega)$ of $C(t)$ by setting it equal to $TX^2_{0\nu}/(z^2_\nu \Delta_\nu)$, where $\Delta_\nu = z_\nu - z_{\nu-1}$, and considering it as a function of $\omega = z_\nu$. This quantity should approach, as $N \to \infty$, the Fourier transform of $C(t)$, which

is given by

$$\tilde{C}(\omega) = T \frac{\kappa\alpha^2/(2\pi)}{(\omega^2 - \omega_0^2)^2(\alpha^2 + \omega^2) + \kappa^2\alpha^4 + 2\kappa\alpha^3(\omega^2 - \omega_0^2)}. \tag{5.3}$$

We will see that the convergence to the large-size irreversible behavior is much slower for the uniform than for the Lorentzian sampling, and that, in the former case, the dynamics seems to remain characterized by underdamped oscillations even at large values of N.

5.1 Sampling

5.1.1 Uniform.

The uniform sampling is obtained by considering N frequencies ω_ℓ ($\ell = 1, 2, \ldots, N$) spaced by a constant Δ. The maximal frequency $N\Delta$ will be denoted by ω_c. The corresponding couplings are given by

$$\epsilon_\ell = \sqrt{\Delta \frac{2}{\pi} \frac{\kappa\alpha^2\omega_\ell^2}{\alpha^2 + \omega_\ell^2}}. \tag{5.4}$$

Then the continuous-limit Ullersma strength is obtained for $N \to \infty$, $\omega_c \to \infty$ and $\Delta = \omega_c/N \to 0$. In this case the Poincaré recurrence time is given by $t_P \simeq 2\pi/\Delta$.

5.1.2 Lorentzian.

In order to obtain a faster convergence with longer Poincaré recurrence times, and a better agreement with the continuum curve both in the under-damping and in the over-damping cases, one can adopt a Lorentzian sampling of frequencies. Positive frequencies distributed with a Lorentzian density centered at $\omega = 0$, with width a_0 are defined as

$$\omega_\ell = a_0 \tan\left[\frac{\ell}{N+1}\frac{\pi}{2}\right], \tag{5.5}$$

with $\ell = 1 \ldots N$ and with the corresponding couplings

$$\epsilon_\ell = \sqrt{\Delta_\ell \frac{2}{\pi} \frac{\kappa\alpha^2\omega_\ell^2}{\alpha^2 + \omega_\ell^2}}, \tag{5.6}$$

where $\Delta_\ell = \omega_\ell - \omega_{\ell-1}$, $\ell = 2, \ldots, N$ and $\Delta_1 = \omega_1$. This sampling enables a high density of frequencies in the area around $\omega = 0$, then determining a long

recurrence time. One can adjust the value of Δ_N in such a way as to have, for all values of N,

$$\sum_\ell \frac{\epsilon_\ell^2}{\omega_\ell^2} = \kappa\alpha. \tag{5.7}$$

We shall refer to this case as the *adjusted Lorentzian* sampling.

5.2 Results

In Figure 5.1 we report the correlation function and the thermal part of second moments of the central oscillator in the classical continuum limit both for an under-damping and an over-damping set of parameters. These are compared with the results obtained in the finite case with $N = 600$ bath particles, both with a uniform and Lorentzian sampling of the bath frequencies. The parameters ω_c and a_0 are chosen so that the Ullersma's spectrum is sampled beyond the cut-off α, and the recurrence time is of the order of the characteristic relaxation time $1/\Gamma$. Finally curves obtained with the adjusted Lorentzian sampling are reported, where the parameter a_0 is chosen so that the recurrence time is much longer than $1/\Gamma$.

In the under-damping case, for a finite bath and for times shorter than the recurrence time, $C(t)$ exhibits the typical damped oscillating behavior of the continuum limit, apart from a shift in the oscillation frequency Ω. On the other hand, $\sigma^2_{q,T}(t)$ and $\sigma^2_{p,T}(t)$ exhibit in the finite-size case the same dissipative behavior as in the continuum case, with a characteristic time $1/\Gamma$. However, while $\sigma^2_{p,T}(t)$ seems to reach, before the Poincaré recurrence time, the same plateau value $k_B T$ as in the continuum case, $\sigma^2_{q,T}(t)$ appears to reach a value lower than the one expected, i.e., $1/(\beta\Omega_0^2)$. These effects are due to the fact that the frequency shift $\sum_\ell \epsilon_\ell^2/\omega_\ell^2$ is different from the continuous limit one $\kappa\alpha$, which appears in Ω_0^2. In fact $\left[\beta\left(\omega_0^2 - \sum_\ell \epsilon_\ell^2/\omega_\ell^2\right)\right]^{-1}$ is equal to the plateau value of $\sigma^2_{q,T}(t)$ reached before the recurrence.

In the over-damping case, as the effect of the frequency shift is larger, one observes a larger difference between the continuum and the finite case. In fact, while the continuum limit curves display the typical over-damped behavior without any oscillations, the finite-case curves exhibit the same behavior observed in the under-damping case. Moreover the difference between the plateau values before the recurrence for $\sigma^2_{q,T}(t)$, is also much larger.

It is clear from Figure 5.1 that with the Lorenzian sampling one obtains curves that behave more similarly to the continuum ones, for the same bath size and recurrence times, with respect to the uniform case. This holds both for the oscillation frequency of $C(t)$ and the plateau value reached by $\sigma^2_{q,T}(t)$ before the recurrence.

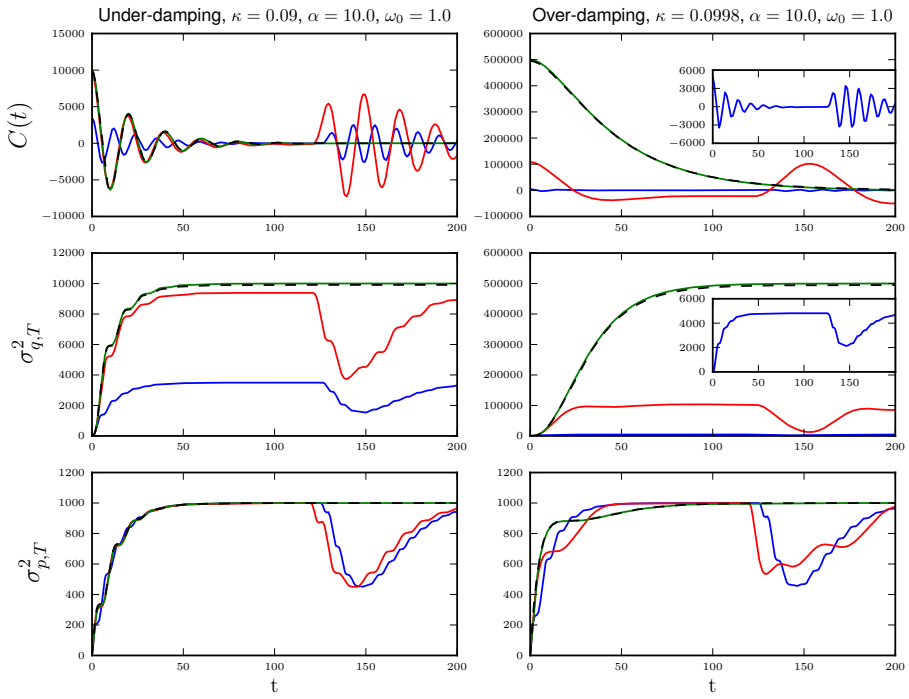

Figure 5.1: Plot of $C(t)$, $\sigma^2_{q,T}(t)$ and $\sigma^2_{p,T}(t)$ in the continuous limit (dashed), compared with the corresponding curves obtained for $N = 600$ with a uniform frequency distribution with $\omega_c = 30.0$ (blue), a Lorentzian distribution of frequencies with $a_0 = 20.0$, (red) and an adjusted Lorentzian distribution with $a_0 = 0.1$ (green). They are obtained both for an under-damping set of parameters (left column) and an over-damping one (right column) in the classical case $T = 1000$. Insets are magnifications of the finite-size curves with uniform sampling.

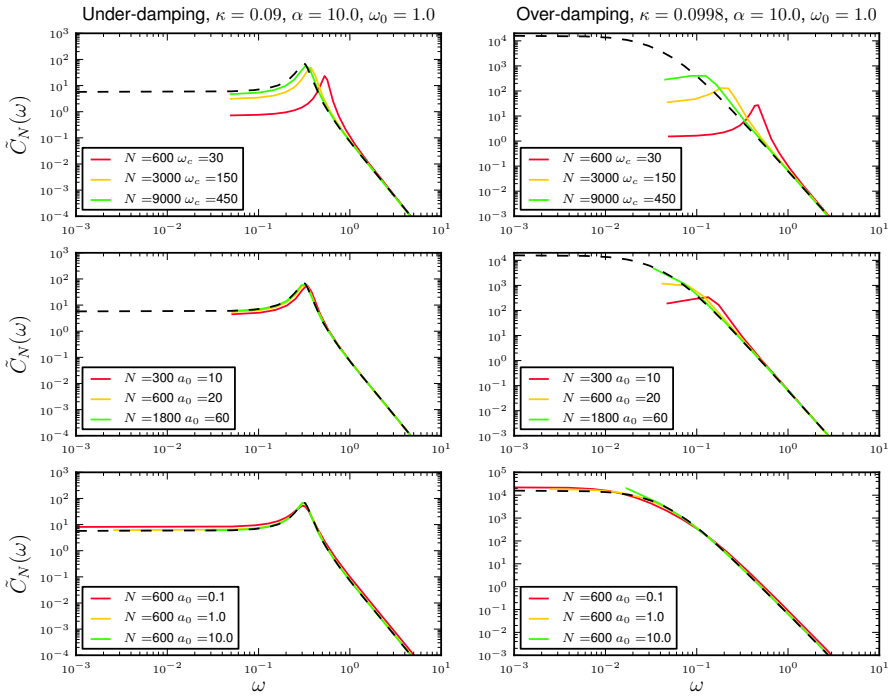

Figure 5.2: Plot of $\tilde{C}_N(\omega)$ vs. ω for different values of the size N of the bath and of the maximal frequancy ω_c (center) or the width a_0, for a uniform (top), Lorentzian (center) and adjusted Lorentzian (bottom) sampling of bath frequencies. The continuum limit $\tilde{C}(\omega)$ corresponds to the dashed line.

One may notice the optimal agreement of the curves obtained with the adjusted Lorentzian distribution with the continuum ones.

The same qualitative behavior of the finite size frequency sampling appear in the Fourier transform of $C(t)$. In Figure 5.2, with the same parameters of Figure 5.1, one notices that in the under-damping regime $\tilde{C}(\omega)$ is characterized by a peak corresponding to the oscillation frequency Ω. A similar curve characterizes $X_{0\nu}^2/(z_\nu^2\Delta_\nu)$, but the position of the peak is shifted. This shift corresponds to the change in the oscillation frequency of $C_N(t)$ with respect to $C(t)$. In the over-damping case the $N = 600$ curve maintains the look of the under-damping case, while the continuous one looses the peak, then confirming that in this case there is a worse agreement between the continuous and the finite cases.

Things improve when ω_c and the size N become larger, keeping the frequency density constant. In this case the peak shifts towards its continuum position in the under-damping case, while in the over-damping case the peak tends to disappear. This improvement is due to the fact that the frequency shift $\sum_\ell \epsilon_\ell^2/\omega_\ell^2$ approaches

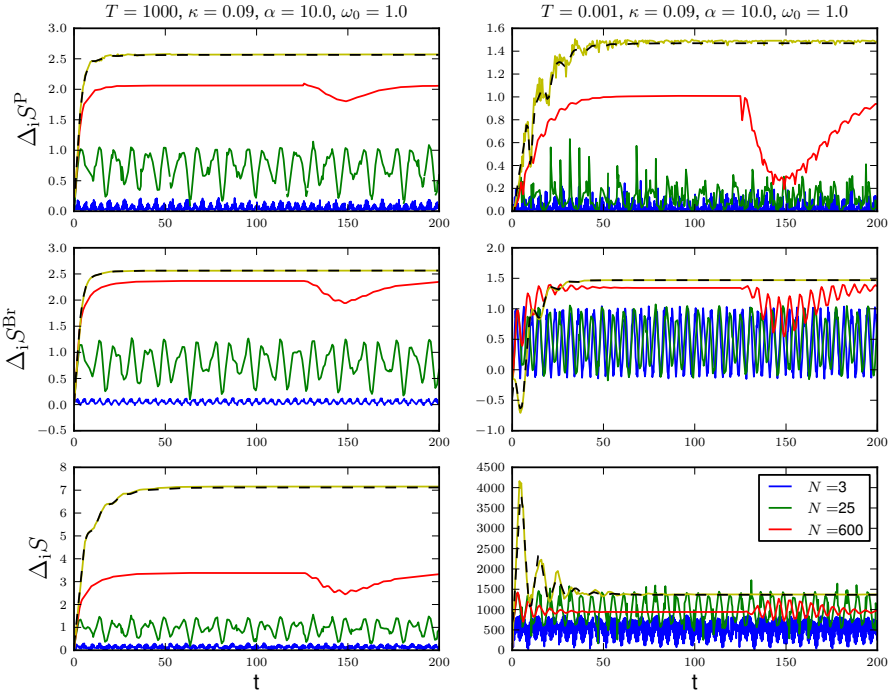

Figure 5.3: Entropy production vs. time t, according to the the three definitions $\Delta_i S^P$, $\Delta_i S^{Br}$ and $\Delta_i S$, for a uniform distribution of bath frequencies with a cut-off $\omega_c = 30$, for different sizes N: 3 (blue), 25 (green), 600 (red), and for the adjusted Lorentzian distribution with $a_0 = 0.1$ (yellow) for $N = 600$. The dashed black line corresponds to the continuum limit. The initial conditions are those of Figure 4.1 in the classical case, apart from the first moments $\left\langle Q^2(0)\right\rangle = 10$ and $\left\langle P^2(0)\right\rangle = 10$, while they are those of Figure 4.2 in the quantum case.

$\int_0^\infty d\omega\, \gamma(\omega)/\omega^2 = \kappa\alpha$. In fact the difference between these quantities is due to two terms: one given by the difference between the sum $\sum_\ell \epsilon_\ell^2/\omega_\ell^2$ and the integral up to ω_c, which is of order $1/N$ and is negligible for the sizes reported in Figure 5.2, and one, more relevant, corresponding to the contribution to the integral arising from frequencies larger than ω_c. This term is proportional to κ. Thus, in order to maintain the difference between $\sum_\ell \epsilon_\ell^2/\omega_\ell^2$ and $\kappa\alpha$ constant, ω_c must increase as κ increases. In particular for a given set of parameters, which would correspond to over-damping in the continuum limit, one would never obtain over-damping behavior if ω_c is too small.

If ω_c or a_0 are kept fixed, and N increases, the behavior remains the same, only the recurrence time t_P increases and the smallest frequency z_1 decreases.

With the Lorentzian sampling of parameters convergence improves both in the

under-damping and in the over-damping cases. In fact, by choosing a_0 and N so that the recurrence time is of the same order as in the uniform case, the value of the frequency shift is closer to $\kappa\alpha$. This is due to the fact that the highest frequency is much larger. One has to exercise some care in choosing a_0 neither too large (in order to have long recurrence times) nor too small (in order to avoid too sparse a sampling close to the highest frequency).

We also show in Figures 5.1 and 5.2 the effect of adjusting the coupling with the highest-frequency oscillator. The behavior of the continuum is optimally matched with the choice $a_0 = 0.1$ and $N = 600$.

5.3 Finite-size entropy production

We report in figure 5.3 the behavior of the entropy production according to the three definitions, i.e., the Poised ($\Delta_{\mathrm{i}}S^{\mathrm{P}}$: eq. (2.9)), the Breuer ($\Delta_{\mathrm{i}}S^{\mathrm{Br}}$: eq. (2.15)) and the ELB ($\Delta_{\mathrm{i}}S$: eq. (2.17)), for different values of N in the uniform case and for $N = 600$ for the adjusted Lorentzian cases. One notices that in the adjusted Lorentzian case one reaches an almost perfect agreement with the continuum limit already for $N = 600$. In the quantum case the expression of the entropy production $\Delta_{\mathrm{i}}S$ obtained with the adjusted Lorentzian binning does not approximate perfectly the continuum limit. This is due to the poor convergence of the term $\langle Q(t)\eta(t)\rangle$ which is contained in the averaged interaction energy $\langle H_I\rangle$ (A.39). The same can be observed for ΔS_i^{P}, due to the noisy behavior of $\dot{A}(t)$ and $\ddot{A}(t)$. At finite sizes the Breuer expression $\Delta_{\mathrm{i}}S^{\mathrm{Br}}$ can assume negative values, whereas both $\Delta_{\mathrm{i}}S$ and $\Delta_{\mathrm{i}}S^{\mathrm{P}}$ remain positive. However, in the uniform case one obtains a slower convergence with respect to the Lorentzian case, both in the adjusted and in the non-adjusted case (not shown).

Chapter 6

Bath entropy

The bath entropy at time t is given by

$$S_{\mathrm{B}}(t) = -\mathrm{tr}\rho_{\mathrm{B}}(t)\ln\rho_{\mathrm{B}}(t), \tag{6.1}$$

where $\rho_{\mathrm{B}}(t) = \mathrm{tr}_{\mathrm{S}}\rho(t)$ is the reduced bath density matrix. Since the total density matrix is not a product state $\rho_{\mathrm{S}}\otimes\rho_{\mathrm{B}}$ at times $t > 0$, one cannot simply split the total entropy into system entropy plus bath entropy. Thus one introduces the correlation entropy S_{c}:

$$S_{\mathrm{tot}} = -\mathrm{tr}\rho(t)\ln\rho(t) = S(t) + S_{\mathrm{B}}(t) + S_{\mathrm{c}}(t). \tag{6.2}$$

We note that $-S_{\mathrm{c}}(t)$ is the mutual information between the central oscillator and the bath [Nielsen and Chuang, 2000]. Since the total entropy is conserved and the initial correlations vanish, one has $S_{\mathrm{c}}(0) = 0$ and, according to this definition,

$$S_{\mathrm{c}}(t) = -\Delta S(t) - \Delta S_{\mathrm{B}}(t). \tag{6.3}$$

We can easily verify that [Esposito et al., 2010]

$$S_{\mathrm{c}}(t) = -D\left[\rho(t)\middle\|\rho_s(t)\prod_r\rho_r(t)\right] \leq 0. \tag{6.4}$$

Thus the correlation entropy is always negative or zero. By comparing this last equation with eq. (2.17), one finds [Esposito et al., 2010]

$$\Delta_{\mathrm{i}}S(t) + S_{\mathrm{c}}(t) = -\beta\langle\Delta H_{\mathrm{B}}\rangle - \Delta S_{\mathrm{B}}(t) = D[\rho_{\mathrm{B}}(t)\|\rho_{\mathrm{B}}^{\mathrm{eq}}] \geq 0. \tag{6.5}$$

One notices that if the approximation of a bath remaining at equilibrium (ideal bath) were valid, i.e., $\rho_{\mathrm{B}}(t) = \rho_{\mathrm{B}}^{\mathrm{eq}}$, the correlation entropy would be equal to minus the entropy production $S_{\mathrm{c}}(t) = -\Delta_{\mathrm{i}}S(t)$. In this case the variation of the bath entropy would be equal to the heat flow.

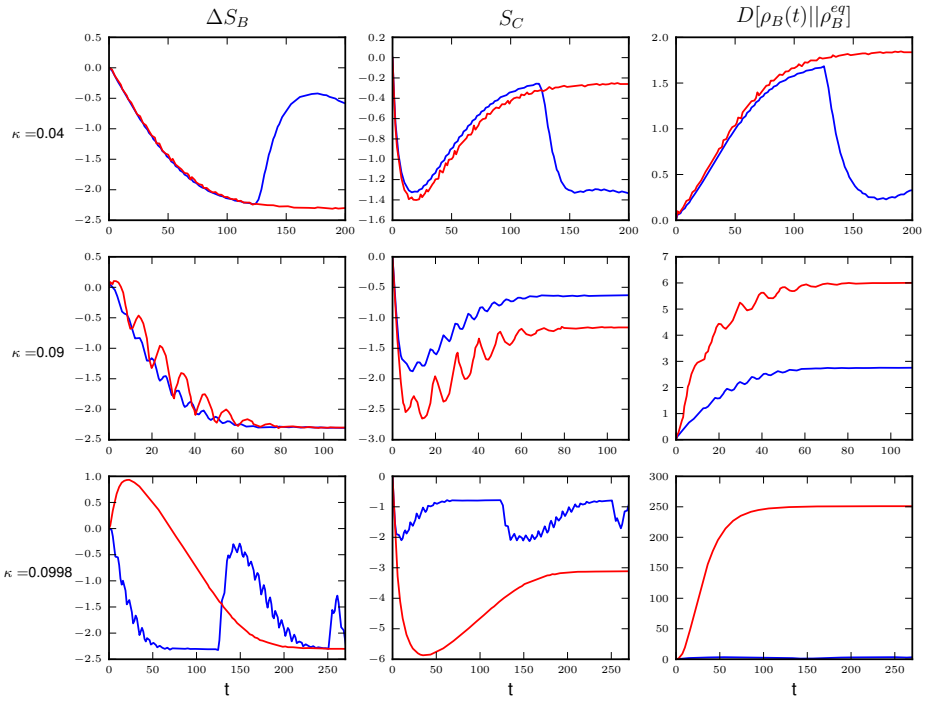

Figure 6.1: Entropy change in the bath ΔS_B, correlation entropy S_C and Kulbach-Leibler distance between $\rho_{\rm B}(t)$ and $\rho_{\rm B}^{\rm eq}$ in the high temperature $T = 1000$ regime, for different values of the coupling κ, for a uniform sampling of frequencies with $\omega_c = 30$ (blue), and for a adjusted Lorentzian one with $a_0 = 0.1$ (red). The bath size is $N = 600$ and other relevant parameters are set as for figure (5.3).

The method to numerically evaluate the bath entropy is detailed in A.7. This calculation relies on the fact that the bath density matrix is Gaussian at each time, and therefore is fully characterized by the time-evolving bath covariance matrix (A.8). We now turn to the discussion of the results.

As observed before for the central oscillator entropy, with an adjusted Lorentzian sampling of frequencies the Poincaré recurrence times are much longer, and one can observe a convergence toward an asymptotic plateau of the different quantities, as shown for the classical case in figure 6.1. In particular the asymptotic value of $\Delta S_{\rm B}$ does not depend on the coupling constant κ, while, in agreement with (A.56), it depends on the initial variances of the central system (see A.8). Interestingly, in the over-damping case $\Delta S_{\rm B}$ increases at the beginning, reaching a maximum independently of the initial conditions, before decreasing to the equilibrium value, much as minus the interaction energy (4.9) does (not shown). The relaxation time is longer than that of the central oscillator. This does not happen

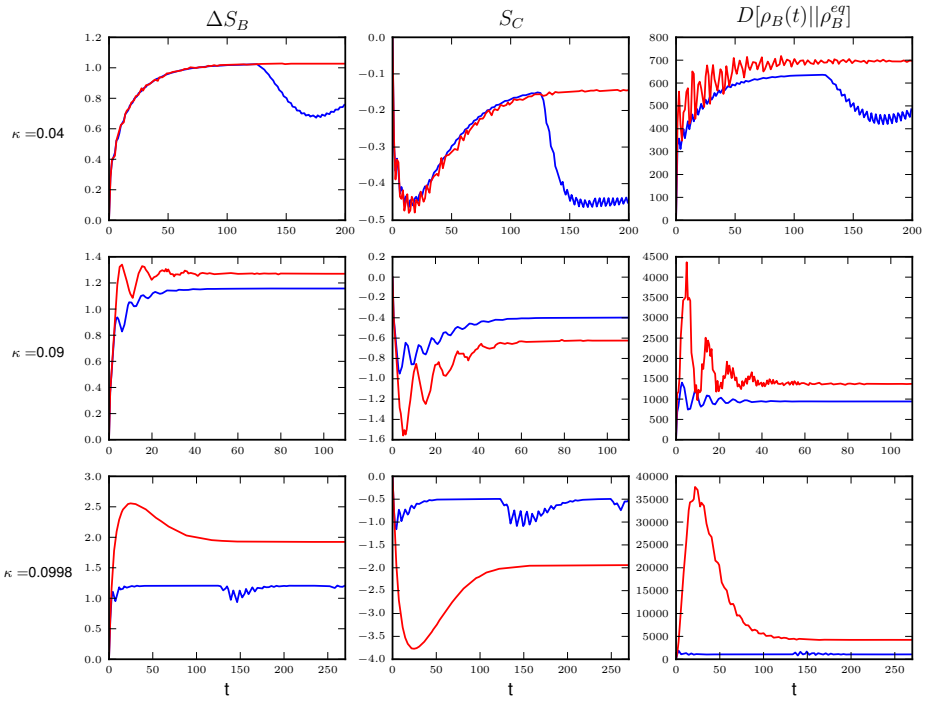

Figure 6.2: Same as figure 6.1 but in the low-temperature case $T = 0.001$, with the other parameters set as in figure 4.2.

in the under-damped regime.

Once the bath entropy ΔS_{B} is evaluated, one also gets the correlation entropy S_{c} using (6.3) and then the distance $D[\rho_{\mathrm{B}}(t)\|\rho_{\mathrm{B}}^{\mathrm{eq}}]$ using (6.5). S_{c} is negative by definition (6.4), and its absolute value grows with the coupling as $-\ln(\omega_0^2 - \kappa\alpha)$, since $\kappa\alpha$ approaches ω_0^2, similarly to the entropy of the system ΔS (4.16). Like the interaction energy term (4.9), the asymptotic value of S_{c} does not depend on the initial conditions of the central system (data not shown). It turns out instead that the asymptotic value of S_{c} vanishes as $\kappa \to 0$. This is confirmed by the fact that the coupling-independent asymptotic value of ΔS_{B} equals minus the central oscillator entropy change in the limit of vanishing coupling:

$$\Delta S_{\mathrm{B}}(\infty) = -\,\Delta S(\infty)|_{\kappa\to 0} = -\left[\ln\frac{T}{\omega_0} - \ln\Delta(0)\right]. \tag{6.6}$$

The distance $D(\rho_{\mathrm{B}}(t)\|\rho_{\mathrm{B}}^{\mathrm{eq}})$ increases with the coupling as $\kappa\alpha/(\omega_0^2 - \kappa\alpha)$, like the negative entropy flow (cf. equation (4.15)). This quantity does not vanish for

$\kappa \to 0$, where it equals the entropy production:

$$\begin{aligned} D(\rho_{\mathrm{B}}(\infty)\|\rho_{\mathrm{B}}^{\mathrm{eq}})\big|_{\kappa\to 0} &= \Delta S_{\mathrm{i}}|_{\kappa\to 0} = [\Delta S(\infty) - \Delta_{\mathrm{e}} S(\infty)]_{\kappa\to 0} \\ &= \ln\frac{T}{\omega_0} - \ln\Delta(0) - \beta\left[T - \frac{1}{2}(\omega_0^2\left\langle Q^2(0)\right\rangle + \left\langle P^2(0)\right\rangle)\right]. \end{aligned} \tag{6.7}$$

As a consequence, the bath density matrix operator is always changed and the Kullback-Leibler distance from the density operator at canonical equilibrium becomes larger when increasing the coupling. This suggests that for our model the ideal bath approximation, namely the assumption $\rho_{\mathrm{B}}(\infty) \simeq \rho_{\mathrm{B}}^{\mathrm{eq}}$, which would imply $\Delta S_{\mathrm{B}} \simeq -\Delta_{\mathrm{e}} S = \beta\Delta\langle H_{\mathrm{B}}\rangle$ (6.5), is not valid even in the thermodynamic limit. One observes in figure 6.2 that in the quantum case the asymptotic value of the bath entropy change appears to grow with the coupling, which could be an effect of the entanglement or quantum correlations between the bath and the system. The dependence on the coupling is apparently weaker than that exhibited by the entropy flow. This means that also here the Kullback-Leibler distance between $\rho_{\mathrm{B}}(t)$ and $\rho_{\mathrm{B}}^{\mathrm{eq}}$ is relevant and strongly increases with the coupling. Due to the quantum contribution in the interaction term, its asymptotic value can be orders of magnitude larger than the one assumed in the high-temperature limit, in the same way ELB entropy production does. In the limit of vanishing coupling analogous considerations of the classical case can be made, since the correlation entropy S_{c} vanishes.

Chapter 7

Two Baths QBM

We consider here the case where the harmonic oscillator is bilinearly coupled to two baths L (left) and R (right) of harmonic oscillators (2.54). The Hamiltonian of the reservoirs and the interaction terms are written as

$$H_{\rm L} = \frac{1}{2}\sum_{i=1}^{N_{\rm L}}\left(\omega_{{\rm L}i}^2 {Q_{{\rm L}i}}^2 + {P_{{\rm L}i}}^2\right),\; H_{\rm R} = \frac{1}{2}\sum_{i=1}^{N_{\rm R}}\left(\omega_{{\rm R}i}^2 {Q_{{\rm R}i}}^2 + {P_{{\rm R}i}}^2\right),$$
$$H_{\rm IL} = \sum_{i=1}^{N_{\rm L}} \epsilon_{{\rm L}i} Q_0 Q_{{\rm L}i}, \quad H_{\rm IR} = \sum_{i=1}^{N_{\rm R}} \epsilon_{{\rm R}i} Q_0 Q_{{\rm R}i}. \tag{7.1}$$

The Heisenberg solutions for the left and right reservoir particles and for the central oscillator reads as in the single bath case (3.3). In this case functions $A_{\mu\nu}(t)$, with indexes $\mu, \nu = 0, \ldots N_{\rm L} + N_{\rm R}$, can be expressed in terms of the function:

$$g(z) = z^2 - \omega_0^2 - \sum_{i=1}^{N_{\rm L}} \frac{\epsilon_{{\rm L}i}^2}{z^2 - \omega_{{\rm L}i}^2} - \sum_{i=1}^{N_{\rm R}} \frac{\epsilon_{{\rm R}i}^2}{z^2 - \omega_{{\rm R}i}^2}, \tag{7.2}$$

whose zeros are the $1 + N_{\rm L} + N_{\rm R}$ normal frequencies of the total Hamiltonian (7.1).

From (7.2) one gets the condition to be fulfilled in order to obtain a positive definite Hamiltonian:

$$\Omega_0^2 = \omega_0^2 - \sum_{i=1}^{N_{\rm L}} \frac{\epsilon_{{\rm L}i}^2}{\omega_{{\rm L}i}^2} - \sum_{i=1}^{N_{\rm R}} \frac{\epsilon_{{\rm R}i}^2}{\omega_{{\rm R}i}^2} \geq 0. \tag{7.3}$$

By using the Heisenberg solutions for the baths position operators as function of the solution for the central oscillator, one finds that the central oscillator satisfies a Quantum Langevin Equation (QLE) of the same form as in the single bath case (3.10): noise in matrix $\boldsymbol{H}(t)$ (3.11) is now $\boldsymbol{\eta}^{\mathsf{T}}(t) = (0, \eta(t) = \eta_{\rm L}(t) + \eta_{\rm R}(t))$ with

component $\eta(t)$ being just the sum of the components associated to the two baths

$$\eta_{\mathrm{L}}(t) = \sum_{i=1}^{N_{\mathrm{L}}} \epsilon_{\mathrm{L}i} \left[Q_{\mathrm{L}i}(0) \cos \omega_{\mathrm{L}i} t + \frac{P_{\mathrm{L}i}(0)}{\omega_{\mathrm{L}i}} \sin \omega_{\mathrm{L}i} t \right], \tag{7.4}$$
$$\eta_{\mathrm{R}}(t) = \sum_{i=1}^{N_{\mathrm{R}}} \epsilon_{\mathrm{R}i} \left[Q_{\mathrm{R}i}(0) \cos \omega_{\mathrm{R}i} t + \frac{P_{\mathrm{R}i}(0)}{\omega_{\mathrm{R}i}} \sin \omega_{\mathrm{R}i} t \right].$$

This holds also for the damping kernel $K(t)$ which becomes the sum of the two following components:

$$K_{\mathrm{L}}(t) = \int_0^\infty \mathrm{d}\omega \, \frac{\gamma_{\mathrm{L}}(\omega)}{\omega^2} \cos \omega t, \quad K_{\mathrm{R}} = \int_0^\infty \mathrm{d}\omega \, \frac{\gamma_{\mathrm{R}}(\omega)}{\omega^2} \cos \omega t, \tag{7.5}$$

where $\gamma_{\mathrm{L}}(\omega)$ and $\gamma_{\mathrm{R}}(\omega)$ is the coupling strengths to the L and R reservoirs:

$$\gamma_{\mathrm{L}}(\omega) = \sum_{i=1}^{N_{\mathrm{R}}} \epsilon_{\mathrm{L}i}^2 \, \delta(\omega - \omega_{\mathrm{L}i}), \quad \gamma_{\mathrm{R}}(\omega) = \sum_{i=1}^{N_{\mathrm{R}}} \epsilon_{\mathrm{R}i}^2 \, \delta(\omega - \omega_{\mathrm{R}i}). \tag{7.6}$$

Also the forcing term $\mathbf{F}(t) = (0, K(t)Q(0))$ contains the new damping kernel. The solution of the QLE has then the same form (3.15) with different noise $\boldsymbol{\eta}(t)$ and matrix propagator $\boldsymbol{\Phi}(t)$. In fact the Laplace transform of $A(t)$ is given by

$$\widehat{A}(s) = \frac{1}{s^2 + s\widehat{K}(s) + \Omega_0^2}, \qquad \widehat{K}(s) = \widehat{K}_{\mathrm{L}}(s) + \widehat{K}_{\mathrm{R}}(s). \tag{7.7}$$

As in the single-bath case all the moments of the total system can be determined analytically.

7.1 Initial conditions and evolution

Given initial conditions (2.55), we are going to restrict to a Gaussian density matrix for the central oscillator. Density matrices of the central system and the reservoirs are both Gaussian, so that they are completely defined by first and second moments of momentum and position operators. The covariance matrix and first moments of the central system S are chosen arbitrarily, and for the baths L and R we have:

$$\begin{aligned}
&\langle Q_{\mathrm{L}i}(0) \rangle = \langle P_{\mathrm{L}i}(0) \rangle = \langle \{ Q_{\mathrm{L}i}(0), P_{\mathrm{L}i}(0) \} \rangle = 0, \\
&\left\langle Q_{\mathrm{L}i}^2(0) \right\rangle = E(\omega_{\mathrm{L}i}, T_{\mathrm{L}}) \ , \ \left\langle P_{\mathrm{L}i}^2(0) \right\rangle = \frac{E(\omega_{\mathrm{L}i}, T_{\mathrm{L}})}{\omega_{\mathrm{L}i}^2}, \\
&\langle Q_{\mathrm{R}i}(0) \rangle = \langle P_{\mathrm{R}i}(0) \rangle = \langle \{ Q_{\mathrm{R}i}(0), P_{\mathrm{R}i}(0) \} \rangle = 0, \\
&\left\langle Q_{\mathrm{R}i}^2(0) \right\rangle = E(\omega_{\mathrm{R}i}, T_{\mathrm{R}}) \ , \ \left\langle P_{\mathrm{R}i}^2(0) \right\rangle = \frac{E(\omega_{\mathrm{R}i}, T_{\mathrm{R}})}{\omega_{\mathrm{R}i}^2}.
\end{aligned} \tag{7.8}$$

Similarly to the single-bath case, due to linearity of evolution and the initial absence of correlations between the central system and the reservoirs, the reduced Wigner satisfies an equation of the form (3.25). The *pseudo-Hamiltonian* $\mathcal{H}(t)$ (3.26) and *diffusion* $\boldsymbol{D}(t)$ (3.27) matrices depends now on a different propagator $A(t)$ (7.7), and a different noise Kernel

$$\begin{aligned} \nu(t) &= \frac{1}{2}\langle\{\eta_{\rm L}(t),\eta_{\rm L}(0)\}\rangle + \frac{1}{2}\langle\{\eta_{\rm R}(t),\eta_{\rm R}(0)\}\rangle = \\ &= \int_0^\infty {\rm d}\omega\, \frac{\gamma_{\rm L}(\omega)}{\omega^2}\, E(\omega,T_{\rm L})\,\cos\omega t + \int_0^\infty {\rm d}\omega\, \frac{\gamma_{\rm R}(\omega)}{\omega^2}\, E(\omega,T_{\rm R})\,\cos\omega t, \end{aligned} \tag{7.9}$$

so that the thermal covariance matrix $\boldsymbol{\sigma}_{\rm TLR}(t)$ (3.28) depends from the two bath temperatures

$$\begin{aligned} \boldsymbol{\sigma}_{\rm TLR}(t) &= \int_0^\infty {\rm d}\omega\, \left[\frac{\gamma_{\rm L}(\omega)}{\omega^2}\, E(\omega,T_{\rm L}) + \frac{\gamma_{\rm R}(\omega)}{\omega^2}\, E(\omega,T_{\rm R})\right]\times \\ &\times\left[\begin{array}{cc} \left|\int_0^t {\rm d}t'\; A(t'){\rm e}^{i\omega t'}\right|^2 & \frac{1}{2}\frac{\rm d}{{\rm d}t}\left|\int_0^t {\rm d}t'\; A(t'){\rm e}^{{\rm i}\omega t'}\right|^2 \\ \frac{1}{2}\frac{\rm d}{{\rm d}t}\left|\int_0^t dt' A(t'){\rm e}^{{\rm i}\omega t'}\right|^2 & \left|\int_0^t {\rm d}t'\; \dot{A}(t'){\rm e}^{{\rm i}\omega t'}\right|^2 \end{array}\right]. \end{aligned} \tag{7.10}$$

Then the solution for the reduced Wigner in Fourier space has the form (3.31), with $\boldsymbol{\sigma}_{\rm TLR}(t)$ in place of $\boldsymbol{\sigma}_T(t)$. Since it is initially Gaussian, it remains Gaussian at later times, so that it is specified by first and second moments of the momentum and position operators:

$$\langle z(t)\rangle = \boldsymbol{\Phi}(t) z_0; \tag{7.11}$$

$$\boldsymbol{\sigma}(t) = \boldsymbol{\Phi}(t)\boldsymbol{\sigma}_0\boldsymbol{\Phi}^{\rm T}(t) + \boldsymbol{\sigma}_{\rm TLR}(t). \tag{7.12}$$

The covariance matrix is the sum of a part depending from initial conditions of the central system, and the thermal covariance part (7.11).

7.2 Thermodynamic limit

The thermodynamic limit of an infinite number of bath oscillators is obtained by substituting continuous function $\gamma_{\rm L}(\omega)$ and $\gamma_{\rm R}(\omega)$ respectively to the discrete coupling strengths of the left and right reservoirs (3.14). We use in both cases a Drude-like Ullersma coupling strength

$$\gamma_{\rm L}(\omega) = \frac{2}{\pi}\frac{\kappa_{\rm L}\alpha^2\omega^2}{\alpha^2+\omega^2}, \qquad \gamma_{\rm R}(\omega) = \frac{2}{\pi}\frac{\kappa_{\rm R}\alpha^2\omega^2}{\alpha^2+\omega^2}. \tag{7.13}$$

The parameters $\kappa_{\rm L}$ and $\kappa_{\rm R}$ tune the strength of the coupling to the two reservoirs, while the cut-off α, can be associated to the bath memory time. For simplicity we

choose it to be equal for the two baths, since we are going still to consider a large cut-off limit, so that we are not interested in what happens for $t < \alpha$. Therefore the damping kernel (3.13) is

$$K(t) = \kappa_{\rm L}\alpha\, {\rm e}^{-\alpha t} + \kappa_{\rm R}\alpha\, {\rm e}^{-\alpha t}, \tag{7.14}$$

and thus decays over times of order α^{-1}.

The general form of the propagator $A(t)$ following from the strength (7.13) remains the same as in the single-bath case. It is characterized by the three time scales Γ, Ω and Λ which can be found from equations (3.36), after replacing $\kappa = \kappa_{\rm L} + \kappa_{\rm R}$, so that the damping over the central system depends from the sum of the couplings to the two baths. In particular in the large cut-off limit

$$\alpha \gg \kappa_{\rm L} + \kappa_{\rm R}, \omega_0. \tag{7.15}$$

it keeps the form of the Ornestein Uhlenbeck propagator (3.40), and one can approximate

$$\lambda \simeq \alpha \ , \ \Gamma \simeq (\kappa_{\rm L} + \kappa_{\rm R})/2 \ , \ \Omega_0^2 \simeq \Gamma^2 + \Omega^2, \tag{7.16}$$

The *pseudo-diffusion* matrix splits into two parts

$$\boldsymbol{D}(t) = \frac{\kappa_{\rm L}}{\kappa_{\rm L} + \kappa_{\rm R}} \boldsymbol{D}_{\rm L}(t) + \frac{\kappa_{\rm R}}{\kappa_{\rm L} + \kappa_{\rm R}} \boldsymbol{D}_{\rm R}(t), \tag{7.17}$$

as well as the thermal covariance matrix

$$\sigma_{\rm TLR}(t) = \frac{\kappa_{\rm L}}{\kappa_{\rm L} + \kappa_{\rm R}} \sigma_{T_{\rm L}}(t) + \frac{\kappa_{\rm R}}{\kappa_{\rm L} + \kappa_{\rm R}} \sigma_{T_{\rm R}}(t), \tag{7.18}$$

where the diffusion matrices $\boldsymbol{D}_{\rm L}(t)$, $\boldsymbol{D}_{\rm R}(t)$ and the thermal covariance matrices $\sigma_{T_{\rm L}}(t)$ and $\sigma_{T_{\rm R}}(t)$ have exactly the same form as in the single bath case (A.41)(A.12) apart from the fact that time scales Ω and Γ depends now from the coupling $\kappa = \kappa_{\rm L} + \kappa_{\rm R}$.

Basically one can consider here the limits:

The low-temperature limit:

$$\alpha \gg 1/\tau_{\beta_{\rm L}}, 1/\tau_{\beta_{\rm R}}; \tag{7.19}$$

The high-temperature classical limit:

$$1/\tau_{\beta_{\rm L}}, 1/\tau_{\beta_{\rm R}} \gg \alpha; \tag{7.20}$$

The weak-coupling limit:

$$\Gamma \ll \Omega, 1/\tau_{\beta_{\rm L}}, 1/\tau_{\beta_{\rm R}}. \tag{7.21}$$

where the thermal transients for the noise kernels of the two reservoirs (7.9) $1/\tau_{\beta_{\rm L}} =$, $1/\tau_{\beta_{\rm R}} =$ are defined. Other possible combinations are due to the fact that couplings and temperatures are different, so one may have one bath strongly coupled and the other weakly, or one classical bath and the other quantum.

Late-time covariance matrix

The late-time moments which characterize the steady state are the weighted sum of the equilibrium moments of the single-reservoir case:

$$\left\langle Q^2(\infty)\right\rangle = \left\langle Q^2\right\rangle_{\rm ss} = \frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}}\left\langle Q^2\right\rangle_{{\rm eq},T_{\rm L}} + \frac{\kappa_{\rm R}}{\kappa_{\rm L}+\kappa_{\rm R}}\left\langle Q^2\right\rangle_{{\rm eq},T_{\rm R}} \tag{7.22}$$

$$\left\langle P^2(\infty)\right\rangle = \left\langle Q^2\right\rangle_{\rm ss} = \frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}}\left\langle P^2\right\rangle_{{\rm eq},T_{\rm L}} + \frac{\kappa_{\rm R}}{\kappa_{\rm L}+\kappa_{\rm R}}\left\langle P^2\right\rangle_{{\rm eq},T_{\rm R}}, \tag{7.23}$$

where the analytical expression for the average squared position and momentum operators at equilibrium are given in (A.19)(A.20). Similarly to the single bath case (3.52), the corresponding Gaussian steady-state density matrix can be put in the form

$$\rho_{\rm S}(\infty) = \rho_{\rm S}^{\rm ss} = \frac{e^{-\phi_{\rm S}^{\rm ss}}}{Z_{\rm S}^{\rm ss}}\ , Z_{\rm S}^{\rm ss} = {\rm tr}_{\rm S} e^{-\phi_{\rm S}^{\rm ss}}, \tag{7.24}$$

where the quadratic operator $\phi_{\rm S}^{\rm ss}$ is given by

$$\phi_{\rm S}^{\rm ss} = \frac{1}{2\phi_1}P^2 + \frac{1}{2}\phi_1\phi_2^2 Q^2. \tag{7.25}$$

The coefficients ϕ_1 and ϕ_2 are expressed as

$$\phi_1 = \frac{1}{\phi_2}\sqrt{\frac{\langle P^2\rangle_{\rm ss}}{\langle Q^2\rangle_{\rm ss}}}\ ,\ \ \phi_2 = \frac{2}{\hbar}\coth^{-1}\left(\frac{2}{\hbar}\sqrt{\langle Q^2\rangle_{\rm ss}\langle P^2\rangle_{\rm ss}}\right), \tag{7.26}$$

where terms $\left\langle Q^2\right\rangle_{\rm ss}$ and $\left\langle P^2\right\rangle_{\rm ss}$ are given in (7.22).

7.3 ELB entropy production rate

In the following we recover an analitic expression for the entropy flow rate $\dot{S}_{\rm e}(t)$. By using the Heisenberg equations for left bath oscillators:

$$\dot{Q}_{{\rm L}i} = P_{{\rm L}i}, \qquad \dot{P}_{{\rm L}i} = -\omega_{{\rm L}i}^2 Q_{{\rm L}i}(t) - \epsilon_{{\rm L}i}Q(t) \tag{7.27}$$

the time derivative of the averaged left reservoir energy $H_{\rm L}(t)$ can be written as :

$$\left\langle \dot{H}_{\rm L}(t)\right\rangle = -\sum_{i=1}^{N_{\rm L}} \epsilon_{{\rm L}i}\left\langle P_{{\rm L}i}(t)Q_0(t)\right\rangle. \tag{7.28}$$

A similar expression holds for the time derivative of the right reservoir energy $H_{\rm R}(t)$.

Moreover we define the average energy current $J_{\rm L}(t)$ from the left reservoir to the central oscillator as:

$$J_{\rm L}(t) = -\left\langle \sum_i \epsilon_{{\rm L}i} P(t) Q_{{\rm L}i}(t) \right\rangle . \tag{7.29}$$

Then by using (7.29) and (7.28), one finds:

$$\left\langle \dot{H}_{\rm L}(t) \right\rangle = -J_{\rm L}(t) - \left\langle \dot{H}_{\rm IL}(t) \right\rangle ,$$

with an analogous expression holding for $\left\langle \dot{H}_{\rm R}(t) \right\rangle$. This means that the entropy flow rate, which is defined as the time-derivative of (2.58), is equal to

$$\dot{S}_{\rm e}(t) = \frac{J_{\rm L}}{T_{\rm L}} + \frac{J_{\rm R}}{T_{\rm R}} + \frac{1}{T_{\rm L}} \left\langle \dot{H}_{\rm IL}(t) \right\rangle + \frac{1}{T_{\rm R}} \left\langle \dot{H}_{\rm IR}(t) \right\rangle , \tag{7.30}$$

which we are able to express explicitly in the large cut-off limit since we have (see (A.67)(A.70)):

$$J_{\rm L}(t) \simeq \frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}} D_{pp,T_{\rm L}}(t) - \kappa_{\rm L} \left\langle P^2(t) \right\rangle + \kappa_{\rm L} \alpha C_{qp}(t) \tag{7.31}$$

$$\left\langle \dot{H}_{\rm IL}(t) \right\rangle \simeq \frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}} \dot{D}_{qp,T_{\rm L}}(t) - 2\kappa_{\rm L} \alpha C_{qp}(t) \tag{7.32}$$

and analogously for $J_{\rm R}$ and $\left\langle \dot{H}_{\rm IR}(t) \right\rangle$, where diffusion coefficients $D_{pp,T_{\rm L}}$ and $D_{qp,T_{\rm L}}$ are the same as in the single-bath case at temperature $T_{\rm L}$ in the large cut-off limit (7.15), with coupling coefficient $\kappa = \kappa_{\rm L} + \kappa_{\rm R}$.

A complete expression for the entropy flow rate is reported in (A.72). In the late-time limit one has

$$\dot{S}_{\rm e}(\infty) = -\dot{S}_{\rm i}(\infty) = \frac{\kappa_{\rm L}\kappa_{\rm R}}{\kappa_{\rm L}+\kappa_{\rm R}} \left[\left\langle P^2 \right\rangle_{{\rm eq},T_{\rm L}} - \left\langle P^2 \right\rangle_{{\rm eq},T_{\rm R}} \right] \left(\frac{1}{T_{\rm L}} - \frac{1}{T_{\rm R}} \right) \tag{7.33}$$

which is always negative, since the average squared momentum at equilibrium (A.20) is an increasing function of the temperature. This was expected, since the late-time value of $\dot{S}_{\rm i}(t)$ has to be positive by definition, in order to guarantee the positivity of $\Delta_{\rm i} S$.

By using general expressions (2.72)(2.73), the 'Breuer' adiabatic and non-adiabatic contributions to ELB entropy production rate $\dot{S}_{\rm i}$ are given by

$$\dot{S}^{\rm Br}_{\rm a}(t) = -\dot{S}_{\rm e}(t) + \left\langle \dot{\phi}^{\rm ss}_{\rm S}(t) \right\rangle , \quad \dot{S}^{\rm Br}_{\rm na}(t) = \dot{S}(t) - \left\langle \dot{\phi}^{\rm ss}_{\rm S}(t) \right\rangle . \tag{7.34}$$

We have used the averaged operator $\phi^{\rm ss}_{\rm S}(t)$ (7.25) and the entropy rate

$$\dot{S}(t) = \dot{\Delta}(t) \ln \frac{\Delta(t) + \frac{1}{2}}{\Delta(t) - \frac{1}{2}}, \tag{7.35}$$

where $\Delta(t)$ was defined in (4.2).

Conclusions

In this work we studied the thermodynamic description of a process of transient relaxation in the QBM model where a central harmonic oscillator initially prepared in a Gaussian nonequilibrium state is bi-linearly coupled with a bath of harmonic oscillators initially prepared at equilibrium.

We compared two ways of defining entropy production during the ensuing relaxation process of the central oscillator. Both definitions are expressed as the difference between the change is the von Neumann entropy of the system minus an heat divided by the temperature of the reservoir. The 'ELB' one is based on defining this heat as minus the energy change in the bath and thus has a straightforward physical interpretation, while the 'Poised' one (beyond non-Markovian transients) defines heat in a less transparent way in term of the change in an effective "mean force" Hamiltonian. Both expressions are positive by definition but in a general non-Markovian quantum regime they both may exhibit oscillations. However, in the Markovian limit, while the 'ELB' may still exhibit oscillations, the 'Poised' one becomes a monotonically increasing function of time. The two definitions coincide for vanishing coupling but we have shown that for finite coupling the 'ELB' is always larger than the 'Poised' one. Their difference contains the expectation value of the interaction Hamiltonian and can thus be made arbitrarily large. In the low-temperature limit the contribution due to the quantum corrections in the interaction term can make this difference order of magnitudes larger than in the classical case. Finally, we showed that in the classical overdamped regime the 'Poised' one converges to the entropy production defined in stochastic thermodynamics.

We numerically studied the exact dynamics of our system for a finite number of oscillators in the bath. Using two different samplings of the bath frequencies, a uniform and a Lorentzian ones. In both cases the period of the Poincaré recurrences increases with growing density of bath frequencies but the Lorentzian sampling guarantees a faster convergence to the continuum limit curves as a function of N.

Finally, we numerically studied the evolution of the von Neumann entropy of the bath which results from the relaxation process of the central oscillator. This

enabled us to calculate the evolution of the system-bath correlation entropy (or minus the mutual information) and the Kullback-Leibler divergence between the bath density matrix at time t and its initial thermal equilibrium form. We observed that for a given initial condition of the central oscillator, the asymptotic value of the bath entropy change does not depend on the coupling in the classical limit, while it slightly does in the quantum regime. In the limit of vanishing coupling strength the correlation entropy vanishes, what means that the change in the von Neumann entropy of the bath becomes equal to minus the change in the central system entropy. We also observed that the Kullback-Leibler divergence of the bath density matrix never vanishes, thus indicating that the assumption of an ideal bath which always remains at equilibrium is not satisfied. As expected, this divergence grows significantly with the coupling, as the ELB expression of the entropy production does.

While our study revealed important features in the QBM model, it also indicates that no definite formulation of a consistent thermodynamics of out-of-equilibrium quantum systems in presence of non-vanishing coupling with the bath is yet available.

In the last chapter we obtained analytical expressions for the entropy production rate for the QBM model with two reservoir. A future work could be a detailed study of the adiabatic and non-adiabatic components of 'ELB' entropy production introduced here.

Another step could be a numerical study of the 'ELB' and 'Lutz' definitions for entropy production in the case work is performed by changing the parameters which characterize the system Hamiltonian or the interaction term, and observing their behavior depending from the velocity of these transormations.

Appendix A

Technical complements

A.1 Equivalence of the Ullersma and Fleming solutions

The convolution with the noise in (3.15) corresponds to the sum over the bath operators in (3.3) and the expression for bath operators in (3.3) correspond exactly to that in (3.9). This equivalence is recovered thanks to the following equation relating the quantities $A_{i0}(t)$ to the propagator $A(t)$, and to the equation relating quantities $A_{ij}(t)$ to $A_{i0}(t)$, where i and j are bath indices:

$$\ddot{A}_{i0}(t) + \omega_i^2 A_{i0}(t) = -\epsilon_i A(t); \tag{A.1}$$

$$\ddot{A}_{ij}(t) + \omega_j^2 A_{ij}(t) = -\epsilon_j A_{i0}(t). \tag{A.2}$$

Given the initial conditions $\dot{A}_{i0}(t) = A_{i0}(t) = A_{ij}(t) = 0$ and $\dot{A}_{ij}(t) = \delta_{ij}$ these equations imply that

$$A_{i0}(t) = -\epsilon_i \int_0^t d\tau A(\tau) \frac{\sin[\omega_i(t-\tau)]}{\omega_i}; \tag{A.3}$$

$$A_{ij}(t) = \frac{\sin(\omega_j t)}{\omega_j}\delta_{ij} - \epsilon_j \int_0^t d\tau A_{i0}(\tau) \frac{\sin[\omega_j(t-\tau)]}{\omega_i}. \tag{A.4}$$

A.2 Covariance matrix

In order to evaluate the covariance matrix of the central oscillator, one evaluates the first and second moments for position and momentum Heisenberg operators. From the Heisenberg solutions (3.3), one obtains by averaging over initial condi-

tions (2.2) (3.19) (3.22) the following expressions:

$$\langle Q(t)\rangle = \dot{A}(t)\langle Q(0)\rangle + A(t)\langle P(0)\rangle\,; \tag{A.5}$$

$$\langle P(t)\rangle = \ddot{A}(t)\langle Q(0)\rangle + \dot{A}(t)\langle P(0)\rangle\,; \tag{A.6}$$

$$\begin{aligned}\sigma_q^2(t) &= \left\langle Q^2(t)\right\rangle - \langle Q(t)\rangle^2 \\ &= \dot{A}^2(t)\sigma_q^2(0) + 2\dot{A}(t)A(t)C_{qp}(0) + A^2(t)\sigma_p^2(0) + \sigma_{q,T}^2(t);\end{aligned} \tag{A.7}$$

$$\begin{aligned}\sigma_p^2(t) &= \left\langle P^2(t)\right\rangle - \langle P(t)\rangle^2 \\ &= \ddot{A}^2(t)\sigma_q^2(0) + 2\ddot{A}(t)\dot{A}(t)C_{qp}(0) + \dot{A}^2(t)\sigma_p^2(0) + \sigma_{p,T}^2(t);\end{aligned} \tag{A.8}$$

$$\begin{aligned}C_{qp}(t) &= \frac{1}{2}\langle\{Q(t) - \langle Q(t)\rangle\,, P(t) - \langle P(t)\rangle\}\rangle \\ &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sigma_q^2(t).\end{aligned} \tag{A.9}$$

The thermal parts of the covariance matrix for a finite bath have the form

$$\sigma_{q,T}^2(t) = \sum_{\ell=1}^{N}\left[\dot{A}_{\ell 0}^2(t)/\omega_\ell^2 + A_{\ell 0}^2(t)\right]E(\omega_\ell, T); \tag{A.10}$$

$$\sigma_{p,T}^2(t) = \sum_{\ell=1}^{N}\left[\ddot{A}_{\ell 0}^2(t)/\omega_\ell^2 + \dot{A}_{\ell 0}^2(t)\right]E(\omega_\ell, T). \tag{A.11}$$

The latter can be also generally written in integral form as shown in (3.30). By combining equations (A.5)-(A.11) one easily obtains also the second moments of the momentum and position operators.

With the continuous bath with the Ullersma coupling strength (3.34) and the high cut-off limit (3.38), by inserting (3.40) in the equations (3.30), one obtains

$$\sigma_{q,T}^2(t) = \{1 + a_{\mathrm{loc}}^2(t)\}\left\langle Q^2\right\rangle_{\mathrm{eq}} + A_{\mathrm{loc}}^2(t)\left\langle P^2\right\rangle_{\mathrm{eq}} + 2\left[A_{\mathrm{loc}}(t)\dot{C}(t) - a_{\mathrm{loc}}(t)C(t)\right]; \tag{A.12}$$

$$\begin{aligned}\sigma_{p,T}^2(t) = {}& \Omega_0^4 A_{\mathrm{loc}}^2(t)\left\langle Q^2\right\rangle_{\mathrm{eq}} + \{1 - \dot{A}_{\mathrm{loc}}^2(t)\}\left\langle P^2\right\rangle_{\mathrm{eq}} \\ & + 2\left[\Omega_0^2 A_{\mathrm{loc}}(t)\dot{C}(t) + \dot{A}_{\mathrm{loc}}(t)\ddot{C}(t)\right];\end{aligned} \tag{A.13}$$

where $a_{\mathrm{loc}}(t) = \dot{A}_{\mathrm{loc}}(t) + 2\Gamma A_{\mathrm{loc}}(t)$, and the position equilibrium correlation function (A.14) is given by

$$C(t) = \frac{1}{2}\langle\{Q(t), Q(0)\}\rangle_{\mathrm{eq}} = \int_0^\infty \mathrm{d}\omega\ \frac{\gamma(\omega)}{\omega^2}E(\omega, T)\left|\int_0^\infty \mathrm{d}t'\ A_{\mathrm{loc}}(t')\mathrm{e}^{\mathrm{i}\omega t'}\right|^2; \tag{A.14}$$

$$\int_0^\infty \mathrm{d}t' A_{\mathrm{loc}}(t')\,\mathrm{e}^{\mathrm{i}\omega t'} = \frac{1}{(\Gamma - \mathrm{i}\omega)^2 + \Omega^2}. \tag{A.15}$$

When calculated with $A_{\rm loc}(t)$, it differs from the exact one by corrections of $\mathrm{O}\,(1/\alpha)$:

$$C(t) = \frac{1}{\beta\Omega_0^2} a_{\rm loc}(t) + \frac{\hbar}{2\pi\Omega}\,\mathrm{Im}\left\{\mathrm{e}^{-(\Gamma+i\Omega)t}\left[\psi(1+(\Gamma+i\Omega)\tau_\beta)\right.\right.$$
$$\left.\left. - \psi(1+(\Gamma-i\Omega)\tau_\beta)\right]\right\} + C_{\alpha,\tau_\beta}(t), \tag{A.16}$$

$$C_{\alpha,\tau_\beta}(t) = \kappa\hbar\left[\frac{1}{2\alpha^2}\frac{\cot(\pi\alpha\tau_\beta)\mathrm{e}^{-\alpha t}}{((1+\frac{\Gamma}{\alpha})^2+(\frac{\Omega}{\alpha})^2)((1-\frac{\Gamma}{\alpha})^2+(\frac{\Omega}{\alpha})^2)}\right.$$
$$\left. - \frac{1}{\pi}\sum_{\ell=1}^{\infty}\frac{(\alpha\tau_\beta)^2}{(\alpha\tau_\beta)^2-\ell^2}\frac{\ell\tau_\beta^2\mathrm{e}^{-\ell t/\tau_\beta}}{((\Omega\tau_\beta)^2+(\ell+\Gamma\tau_\beta)^2)((\Omega\tau_\beta)^2+(\ell-\Gamma\tau_\beta)^2)}\right]. \tag{A.17}$$

In this expression, $\psi(z) = \mathrm{d}\ln\Gamma_{\rm E}(z)/\mathrm{d}z$ is the digamma function, and τ_β was defined in 3.43. The last term contains the so called thermal transients, which vanish slowly in the low-temperature limit. By discarding terms of $\mathrm{O}\left(1/\alpha^2\right)$, in the quantum limit $\alpha\tau_\beta \gg 1$ it can be approximated for $t \gg 1/\alpha$ by the series [Haake and Reibold, 1985]

$$C_{\alpha,\tau_\beta}(t) \simeq \frac{\hbar}{\pi\Omega}\,\mathrm{Im}\sum_{\ell=1}^{\infty}\frac{\ell\mathrm{e}^{-\ell t/\tau_\beta}}{(\Gamma+i\Omega)^2\tau_\beta^2-\ell^2}. \tag{A.18}$$

One should remark however that its second time derivative diverges at $t = 0$, and that other terms should be taken in account in order to remove this divergence. We truncate this sum to 50 terms, what guarantees a good description for $t \gg 1/\alpha$. One has however to take into account the fact that our approximations do not describe well the behavior for $t \leq 1/\alpha$.

The equilibrium second moments one gets from the equilibrium correlation function (A.14) at $t = 0$ are given by [Haake and Reibold, 1985]

$$\left\langle Q^2\right\rangle_{\rm eq} = C(0) = \frac{T}{\Omega_0^2} + \frac{\hbar}{\pi\Omega}\,\mathrm{Im}\,\psi(1+(\Gamma+i\Omega)\tau_\beta); \tag{A.19}$$

$$\left\langle P^2\right\rangle_{\rm eq} = -\ddot{C}(0) = T + \frac{2}{\pi}\hbar\Gamma\,\mathrm{Re}\left(\ln\alpha\tau_\beta - \psi(1+(\Gamma+i\Omega)\tau_\beta)\right)$$
$$+ \frac{\hbar(\Omega^2-\Gamma^2)}{\pi\Omega}\,\mathrm{Im}\,\psi(1+(\Gamma+i\Omega)\tau_\beta). \tag{A.20}$$

Here the average is carried over the equilibrium density matrix $\rho^{\rm eq}$ (3.52). This time, in order to correctly evaluate $\left\langle P^2\right\rangle_{\rm eq}$ to $\mathrm{O}\,(1/\alpha)$, one has to consider all the terms contained in $C_{\alpha,\tau_\beta}(t)$. One should keep in mind that $\left\langle P^2\right\rangle_{\rm eq}$ contains a contribution $\ln\alpha/\nu$, what explains the necessity of introducing a high-frequency cut-off.

A.3 Effect of initial slips

As we have recalled in section (3.3), slips in the averaged momentum operator and in the correlation matrix are produced by the kick-like force term $F(t)$ in the QLE (3.10), acting during an inital time interval of duration $\sim 1/\alpha \simeq 1/\lambda$. The local propagator (3.40) actually contains such slips from $t = 0^+$, so that it is correct apart from corrections of $\mathrm{O}(1/\lambda)$ only for $t \gg 1/\lambda$ (see eq. 3.47), namely when the kick vanishes. In fact, while $A(0)$ contains corrections of the kind $(1/\lambda^2)\mathrm{e}^{-\lambda t}$ with respect to $A_{\mathrm{loc}}(0)$, its second time derivative contains a term $\mathrm{e}^{-\lambda t}$, so that it is negligible only for $t \gg 1/\lambda$. With the local propagator (3.40) we are not going to consider the detail of the evolution in the initial time interval of duration $1/\alpha$, which is considered to be much shorter than the other time scales in the large cut-off limit.

The initial slips correspond to a fast shift of the initial conditions:

$$\begin{aligned}
&\langle P(0)\rangle \to -2\Gamma\langle Q(0)\rangle + \langle P(0)\rangle\,;\\
&\left\langle P^2(0)\right\rangle \to 4\Gamma^2\left\langle Q^2(0)\right\rangle - 2\Gamma\left\langle\frac{\{Q(0),P(0)\}}{2}\right\rangle + \left\langle P^2(0)\right\rangle\,;\\
&\left\langle\frac{\{Q(0),P(0)\}}{2}\right\rangle \to -2\Gamma\left\langle Q^2(0)\right\rangle + \left\langle\frac{\{Q(0),P(0)\}}{2}\right\rangle.
\end{aligned} \tag{A.21}$$

Let us now discuss the effect of the initial slips (A.21) on the Breuer (2.13) and ELB (2.17) entropy definitions. They appear as a nonvanishing value for

$$\lim_{t\to 0^+}\Delta_{\mathrm{e}}S(t) = \Delta_{\mathrm{e}}S(0^+), \qquad \lim_{t\to 0^+}\Delta S(t) = \Delta S(0^+). \tag{A.22}$$

For the Breuer entropy flow one has, by using the expressions of the moments reported in (A.5):

$$\Delta_{\mathrm{e}}S^{\mathrm{Br}}(0^+) = \beta\left[\frac{1}{M_{\mathrm{eff}}}(2\Gamma^2\left\langle Q^2(0)\right\rangle - \Gamma C_{qp}(0))\right], \tag{A.23}$$

which is due to the shift on $\left\langle P^2(0)\right\rangle$. For the entropy change one has

$$\begin{aligned}
\Delta S(0^+) = {}&(\Delta_{is}(0)+1)\ln(\Delta_{is}(0)+1) - \Delta_{\mathrm{is}}\ln\Delta_{\mathrm{is}}\\
&-(\Delta(0)+1)\ln(\Delta(0)+1) - \Delta(0)\ln\Delta(0);
\end{aligned} \tag{A.24}$$

$$\Delta_{\mathrm{is}} = (\sigma_q^2(0)\sigma_p^2(0) - C_{qp}(0)(C_{qp}(0) - 2\Gamma\sigma_q^2(0)))^{\frac{1}{2}} - \frac{1}{2}, \tag{A.25}$$

where $\Delta(0)$ is given in (4.1). $\Delta_{\mathrm{is}} > \Delta(0) \geq 0$ satisfies the Heisenberg principle, and therefore $\Delta S(0^+)$ is always positive.

For the ELB entropy flow one has

$$\Delta_{\mathrm{e}} S(0^+) = \beta \left[2\Gamma^2 \left\langle Q^2(0) \right\rangle - \Gamma C_{qp}(0)) - \kappa\alpha \left\langle Q^2(0) \right\rangle \right]. \tag{A.26}$$

Here the sign is determined by the last term, which is generally larger than the first one, due to the large value assumed by α. In principle one should also consider a slip term $\frac{4}{\pi}\hbar\Gamma\psi(1 + \lambda\tau_\beta)$ in $\left\langle P^2(0) \right\rangle$, because we used the approximate formula (A.18) to calculate (A.13). However, the effect of neglecting this term as well as the effect of the truncation of the sum in (A.18) are negligible compared to the slips considered above.

A.4 Calculation of the Poised entropy production

In order to evaluate the Poised entropy production $\Delta_{\mathrm{i}} S^{\mathrm{P}}$ in eq.(2.9), we have to find the poised density matrix $\rho^*_{\mathrm{S}}(t)$. Once it is known, on can evaluate $\Delta_{\mathrm{i}} S^{\mathrm{P}}$ as

$$\Delta_{\mathrm{i}} S^{\mathrm{P}} = \Delta S - \Delta_{\mathrm{e}} S^{\mathrm{P}} = \Delta S - \mathrm{tr}_{\mathrm{S}} \left(\rho_{\mathrm{S}}(0) - \rho_{\mathrm{S}}(t) \right) \ln \rho^*_{\mathrm{S}}(t). \tag{A.27}$$

In order to evaluate $\rho^*_{\mathrm{S}}(t)$, we rewrite equation $V(t)\rho^*_{\mathrm{S}}(t) = \rho^*_{\mathrm{S}}(t)$ in the Fourier transform space associated with the corresponding Wigner $W^*_{\mathrm{S}}(q, p, t)$. Using eq.(3.31) we get

$$\widetilde{W}^*_{\mathrm{S}}(\boldsymbol{\Phi}^{\mathsf{T}}(t)\boldsymbol{k}, t)\, \mathrm{e}^{-\frac{1}{2}\boldsymbol{k}^{\mathsf{T}}\boldsymbol{\sigma}_T(t)\boldsymbol{k}} = \widetilde{W}^*_{\mathrm{S}}(\boldsymbol{k}, t). \tag{A.28}$$

Since we only consider initial Gaussian distributions, we have seen that the solution remains Gaussian at any time. Therefore, to solve (A.28), we look for solutions of the form

$$\widetilde{W}^*_{\mathrm{S}}(\boldsymbol{k}, t) = \mathrm{e}^{-\frac{1}{2}\boldsymbol{k}^{\mathsf{T}}\boldsymbol{\sigma}^*(t)\boldsymbol{k} - \mathrm{i}\boldsymbol{k}^{\mathsf{T}}\boldsymbol{z}^*(t)}, \tag{A.29}$$

where $\boldsymbol{\sigma}^*(t)$ is a symmetric 2×2 covariance matrix:

$$\boldsymbol{\sigma}^*(t) = \begin{bmatrix} \sigma^{*2}_q(t) & C^*_{qp}(t) \\ C^*_{qp}(t) & \sigma^{*2}_p(t) \end{bmatrix}, \tag{A.30}$$

and the vector $\boldsymbol{z}^*(t)$ contains the first moments $q^*(t)$ and $p^*(t)$. By using expression (A.29) in equation (A.28) one straightforwardly finds the relation between the covariance matrices and the first moments:

$$\boldsymbol{\Phi}(t)\boldsymbol{\sigma}^*(t)\boldsymbol{\Phi}^{\mathsf{T}}(t) + \boldsymbol{\sigma}_T(t) = \boldsymbol{\sigma}^*(t); \tag{A.31}$$

$$\boldsymbol{\Phi}(t)\boldsymbol{z}^*(t) = \boldsymbol{z}^*(t). \tag{A.32}$$

From equation (A.32) one finds $z^*(t) = 0$ at all times. Equation (A.31) for the covariance matrix is equivalent to a system of three equations. One gets

$$\sigma_q^{*2}(t) = \frac{\sigma_{q,T}^2(t)S_{11}(t) + C_{qp,T}(t)S_{12}(t) + \sigma_{p,T}^2(t)S_{13}(t)}{D_{11}(t)D_{12}(t)D_{21}(t)}; \tag{A.33}$$
$$C_{qp}^*(t) = \frac{C_{qp,T}(t)S_{22}(t) + \sigma_{q,T}^2(t)S_{21}(t) + \sigma_{p,T}^2(t)S_{23}(t)}{D_{12}(t)D_{21}(t)};$$
$$\sigma_p^{*2}(t) = \frac{\sigma_{p,T}^2(t)S_{33}(t) + C_{qp,T}(t)S_{32}(t) + \sigma_{q,T}^2(t)S_{31}(t)}{D_{11}(t)D_{12}(t)D_{21}(t)}.$$

Here

$$\begin{aligned}
S_{11} &= S_{33} = 1 - 2\dot{A}^2 + \dot{A}^4 - A\ddot{A} - \dot{A}^2 A\ddot{A}; \\
S_{12} &= -2\dot{A}A(1 - \dot{A}^2 + A\ddot{A}); \\
S_{13} &= -A^2(1 + \dot{A}^2 - A\ddot{A}); \\
S_{21} &= \dot{A}\ddot{A}; \\
S_{22} &= 1 - \dot{A}^2 - A\ddot{A}; \\
S_{23} &= A\dot{A}; \\
S_{31} &= -\ddot{A}^2(1 + \dot{A}^2 - A\ddot{A}); \\
S_{32} &= -2\dot{A}\ddot{A}(1 - \dot{A}^2 + A\ddot{A}); \\
D_{11} &= 1 - \dot{A}^2 + A\ddot{A}; \\
D_{12} &= 1 - 2\dot{A} + \dot{A}^2 - A\ddot{A}; \\
D_{21} &= 1 + 2\dot{A} + \dot{A}^2 - A\ddot{A}.
\end{aligned} \tag{A.34}$$

Thus the elements of the matrix $\boldsymbol{\sigma}^*(t)$ are expressed as linear combinations of thermal covariance elements, whose coefficients are functions of the propagator matrix elements. Expressions (A.33) are valid both in the finite-size case and in the thermodynamic limit. In order to get the poised covariance matrix at $t = 0$ one has to evaluate the $t \to 0^+$ limit of (A.33).

A.5 Liouvillian operator of the adjoint dynamics

In the adjoint dynamics, the system and bath Heisenberg operators satisfy the following equations:

$$\dot{Q}_\mu(t) = -\frac{\mathrm{i}}{\hbar}\Big[H, Q_\mu(t)\Big] \quad , \quad \dot{P}_\mu(t) = -\frac{\mathrm{i}}{\hbar}\Big[H, P_\mu(t)\Big], \tag{A.35}$$

where one has a change of sign respect to the usual Heisenberg dynamics (3.2). By proceeding in the same way as in the usual case, we find the following modifications involving the matrix QLE satisfied by the central oscillator (3.10):

$$\boldsymbol{H}(t) \to \tilde{\boldsymbol{H}}(t) = \begin{bmatrix} 0 & \delta(t) \\ -\Omega_0^2\delta(t) & K(t) \end{bmatrix}, \tag{A.36}$$

$$\eta(t) \to \tilde{\eta}(t) = \sum_i^N \epsilon_i \left[-Q_i(0)\cos\omega_i t + \frac{P_i(0)}{\omega_i}\sin\omega_i t \right]. \tag{A.37}$$

This imply that the evolution is given as in equation (3.15), but with a change in the off-diagonal elements of the matrix propagator (3.16):

$$\boldsymbol{\Phi}(t) \to \tilde{\boldsymbol{\Phi}}(t) = \begin{bmatrix} \dot{A}(t) & -A(t) \\ -\ddot{A}(t) & \dot{A}(t) \end{bmatrix}, \tag{A.38}$$

while the noise kernel (3.42) remains unchanged. By considering the above modifications, one straightforwardly find from (3.25) the FP-like equation satisfied by the reduced Wigner for the central oscillator for the adjoint dynamics: it remains exactly the same except for a change in the signs of the drift term, the harmonic forcing term and the anomalous diffusion coefficient. This imply that the limits generally considered in section (3.3) for the usual process do also apply for the adjoint, moreover the late time density matrix is the same as in (3.3).

In the case of two baths one can show analogously that the same sign changes characterizes the FP-like equation satisfied by the reduced Wigner associated to the global adjoint dynamics. This means that also in this case the usual and adjoint dynamics determine the same steady-state for the central oscillator.

A.6 Interaction energy term

A way to express the average of H_{I}, which is useful in the continuum limit, is the following. By plugging the Heisenberg formal solutions for the bath operators as functions of $Q(t)$ (3.9) in the interaction term, one gets

$$\langle H_{\mathrm{I}}(t)\rangle = \left\langle \sum_i Q(t)Q_i(t) \right\rangle = \langle Q(t)\eta(t)\rangle + \left\langle \int_0^t \mathrm{d}s\ \dot{K}(t-s)Q(t)Q(s) \right\rangle, \tag{A.39}$$

where $\eta(t)$ is the fluctuating force term defined in (3.12).Using (3.15) and the initial absence of system-bath correlation, which implies $\langle Q(0)\eta(t)\rangle = 0$, one gets

$$\begin{aligned} \langle Q(t)\eta(t)\rangle &= -\int_0^t \mathrm{d}t'\ A(t-t')\,\langle \eta(t')\eta(t)\rangle \\ &= -\int_0^\infty \mathrm{d}\omega\ \frac{\gamma(\omega)}{\omega^2}E(\omega,T)\int_0^t \mathrm{d}s\ A(s)\cos(\omega s). \end{aligned} \tag{A.40}$$

Interestingly the use of the Ullerma strength (3.34), from which one obtains that the damping coefficients are time-independent in the large cut-off limit, implies exactly the same integral form for the anomalous diffusion coefficient, so that $\langle Q(t)\eta(t)\rangle = D_{qp}(t)$.

In fact in the case of the Ullersma strength (3.34) with large cut-off the diffusion matrix (3.27) can be approximated by [Fleming et al., 2011]

$$\boldsymbol{D}(t) = \frac{1}{2}\int_0^t \mathrm{d}\tau \, \left[\boldsymbol{\nu}(t-\tau)\boldsymbol{\Phi}^{\mathsf{T}}(t-\tau) + \boldsymbol{\Phi}(t-\tau)\boldsymbol{\nu}^{\mathsf{T}}(t-\tau)\right]. \tag{A.41}$$

This straightforwardly leads to the equivalence between $\langle Q(t)\eta(t)\rangle$, which is part of the average interaction term (4.9), and the anomalous diffusion term $D_{qp}(t)$. The diagonal term $D_{pp}(t)$ of (A.41) results equal to $-\langle P(t)\eta(t)\rangle$, which is calculated later in the appendix (A.69).

The integral (A.40) is done by using the local propagator $A_{\mathrm{loc}}(t)$ (3.40), by first integrating over time and then in the complex ω plane. One obtains

$$D_{qp}(t) = \left\langle P^2\right\rangle_{\mathrm{eq}} - \Omega_0^2\left\langle Q^2\right\rangle_{\mathrm{eq}} - \left\{\dot{A}_{\mathrm{loc}}(t) + A_{\mathrm{loc}}(t)\left(2\Gamma - \frac{d}{dt}\right)\right\} F_C(t); \tag{A.42}$$

$$F_C(t) = -(\ddot{C}(t) + \Omega_0^2 C(t) + 2\Gamma\dot{C}(t)). \tag{A.43}$$

The time dependent term contained in (A.42) vanishes so that one recovers the late-time anomalous diffusion coefficient (3.48), which is a positive quantity. Here we have made use of the approximate equilibrium correlation function (A.16). It follows that

$$F_C(t) = \kappa\hbar\left[-\frac{1}{2}\frac{\cot(\pi\alpha\tau_\beta)\mathrm{e}^{-\alpha t}}{(1+(\Gamma/\alpha))^2 + (\Omega/\alpha)^2} + \frac{1}{\pi}\sum_{\ell=1}^{\infty}\frac{(\alpha\tau_\beta)^2}{(\alpha\tau_\beta)^2 - \ell^2}\frac{\ell\mathrm{e}^{-\ell t/\tau_\beta}}{(\ell+\Gamma\tau_\beta)^2 + (\Omega\tau_\beta)^2}\right], \tag{A.44}$$

which can be approximated for $t \gg 1/\alpha$ by

$$F_C(t) \simeq \frac{\kappa\hbar}{\pi}\sum_{\ell=1}^{\infty}\frac{\ell\mathrm{e}^{-\ell t/\tau_\beta}}{(\ell+\Gamma\tau_\beta)^2 + (\Omega\tau_\beta)^2}. \tag{A.45}$$

In the classical limit the anomalous diffusion coefficient vanishes.

To evaluate the second term of the sum in (A.39), we can use the fact that for large cut-off $\dot{K}(t) \sim -\kappa\alpha\delta(t)$. Then one gets for the interaction term complete expression (4.9).

In the finite case one has, by using the solutions (3.3) and the initial conditions

(2.2):

$$\left\langle \sum_{i=1}^{N} Q(t)Q_i(t) \right\rangle = \sum_{i=1}^{N} \Big\{ \epsilon_i \dot{A}_{00}\dot{A}_{i0} \left\langle Q^2(0) \right\rangle + A_{00}A_{i0} \left\langle P^2(0) \right\rangle + (\dot{A}_{00}A_{i0} + \dot{A}_{i0}A_{00}) C_{qp}(0) + \sum_{j=1}^{N} \left(\frac{\dot{A}_{0i}\dot{A}_{ji}}{\omega_i^2} + A_{0i}A_{ji} \right) E(\omega_i, T) \Big\}. \tag{A.46}$$

This expression is useful for a numerical calculation in the finite case. By using the expression of the $A_{i0}(t)$ and the $A_{ij}(t)$ in function of the propagator $A(t)$, one obtains the expressions (A.39,A.40) exploited in the continuum limit.

A.7 Evaluation of the bath entropy

One can straightforwardly evaluate the general quantum bath entropy (6.1) if one finds a coordinate transformation that puts the density operator ρ_{B} in a normal form, namely a product of independent oscillator thermal states:

$$\rho_{\mathrm{B}} = \bigotimes_{\ell} (1 - \mathrm{e}^{-\beta_\ell}) \, \mathrm{e}^{-\beta_\ell n_\ell}, \tag{A.47}$$

where $n_\ell = a_\ell^\dagger a_\ell$, with $a_\ell = (q_\ell + \mathrm{i}p_\ell)/\sqrt{2}$, and where the β_ℓ are suitable effective inverse temperatures. In fact, by putting the density operator in this form, the calculation of entropy is easily obtained by carrying the trace over the space of the eigenstates of the number operator: $|n_1, n_2, \ldots, n_\ell, \ldots, n_N\rangle$. One obtains

$$S_{\mathrm{B}} = \sum_{\ell} ((k_\ell + 1/2)\ln(k_\ell + 1/2) - (k_\ell - 1/2)\ln(k_\ell - 1/2)), \tag{A.48}$$

where $k_\ell = \frac{1}{2}\coth\left(\frac{1}{2}\beta_\ell\right) = \left\langle q_\ell^2 \right\rangle = \left\langle p_\ell^2 \right\rangle = \langle n_\ell \rangle + \frac{1}{2}$. For simplicity we have put here $\hbar = 1$.

We know from (3.2) that the reduced density matrix for the bath is Gaussian. Here first moments can be shifted to 0, as this transformation leaves the entropy invariant. Then from an informational point of view the bath is fully characterized by the covariance matrix σ_{ij}^{B} (A.59).

The normal form (A.47) and values of the k_ℓ's can be actually recovered by a "pseudo-diagonalization" of the correlation matrix. This can be done using a symplectic transformation, $\xi \mapsto S\xi$ where S is a $2N \times 2N$-matrix, i.e. a transformation preserving the bosonic commutation rules:

$$\boldsymbol{\beta} = S\boldsymbol{\beta}S^{\mathsf{T}}, \tag{A.49}$$

where

$$\boldsymbol{\beta} = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}; \qquad \mathbf{1} = (\delta_{k,\ell}), \quad k, \ell = 1, 2, \ldots, N. \tag{A.50}$$

One then choose S such that the correlation matrix in the new basis is diagonal:

$$\sigma^{\mathrm{B}} \mapsto \sigma'^{\mathrm{B}} = S \sigma^{B} S^{\mathsf{T}} = \mathrm{diag}(\kappa_1, \kappa_2, \ldots, \kappa_N, \kappa_1, \kappa_2, \ldots, \kappa_N). \tag{A.51}$$

This can always be done, as affirmed by Williamson's theorem [Williamson, 1936], due to the fact that the correlation matrix is symmetric and positive definite. Due to the particular block form of the correlation matrix, the k_ℓ's are doubly degenerate, as shown in [Colpa, 1978].

The pseudo-eigenvalues and the symplectic matrix S can be obtained, as explained in [Simon et al., 1994], by diagonalizing the symmetric matrix $K\beta\sigma^{\mathrm{B}}\beta^{\mathsf{T}}K^{\mathsf{T}}$, where the matrix K is obtained by a Cholesky decomposition of the correlation matrix:

$$\sigma^{B} = K^{\mathsf{T}} K. \tag{A.52}$$

This can actually be carried out, since σ^B is positive definite. The eigenvalues one finds are actually the doubly-degenerate squares of the pseudo-eigenvalues k_ℓ.

Given an operator $\hat{A}$, its Wigner transform is defined by [Hillery et al., 1984]

$$A(p, q) = \int \mathrm{d}z \; \mathrm{e}^{\mathrm{i}pz/\hbar} \left\langle q - \frac{z}{2} \middle| \hat{A} \middle| q + \frac{z}{2} \right\rangle. \tag{A.53}$$

In the general quantum case, the Wigner transform of $\ln \rho_{\mathrm{B}}$ is $-\xi^{\mathsf{T}} M \xi - \ln Z_{\mathrm{B}}$, since one has

$$\rho_{\mathrm{B}} = \exp\{-\xi^{\mathsf{T}} M \xi\}/Z_{\mathrm{B}}, \tag{A.54}$$

where M is a square $2N \times 2N$ matrix. This matrix transforms under a symplectic transformation of the phase space operators (A.49) like $(\sigma^{\mathrm{B}})^{-1}$:

$$M \mapsto M' = (S^{\mathsf{T}})^{-1} M S^{-1}. \tag{A.55}$$

In the classical limit the diagonalized matrices M' and $(\sigma'^{\mathrm{B}})^{-1}$, coincide and therefore also $(\sigma^{B})^{-1}$ and M have to coincide. Therefore in the classical limit the Wigner distribution corresponding to the density operator ρ_{B} has the same expression as the classical probability distribution apart from multiplicative coefficients, i.e.,

$$W_{\mathrm{B}}(q, p, t) = \exp\{-\frac{1}{2}\xi^{\dagger}(\sigma^{\mathrm{B}})^{-1}\xi\} / \left[(2\pi)^N (\det \sigma^{\mathrm{B}})^{1/2}\right]. \tag{A.56}$$

where σ^{B} is given in eq. (A.59). Then the entropy of the bath can be easily calculated via a Gaussian integral:

$$\begin{aligned} S_{\mathrm{B}} &= -\int \mathrm{d}q \, \mathrm{d}p \; W_{\mathrm{B}}(q, p, t)_{\mathrm{CL}} \ln\left[(2\pi)^N W_{\mathrm{B}}(q, p, t)_{\mathrm{CL}}\right] \\ &= N + \ln(\det \sigma^{\mathrm{B}})^{1/2}. \end{aligned} \tag{A.57}$$

This result can be also be obtained by noticing that in the classical limit, where $k_\ell \gg \hbar/2$, the expression (A.48) for the bath entropy reduces to

$$S_{\rm B} = N + \ln \prod_{\ell=1}^{N} k_\ell = N + \ln(\det S\, \sigma^B S^{\mathsf{T}})^{1/2}. \tag{A.58}$$

Thus, since $\det S = 1$ (A.49) we recover (A.57).

A.8 Bath covariance matrix

The covariance matrix of the bath is defined as:

$$\sigma^{\rm B}_{ij} = \frac{1}{2}\langle\{\xi_i, \xi_j\}\rangle - \langle\xi_i\rangle\langle\xi_j\rangle, \tag{A.59}$$

where $\xi = (Q_1, ..., Q_N, P_1, ..., P_N)$, i and j identify the bath oscillators.

Using the Heisenberg solutions (3.3), the variance of a bath position operator with average taken over the initial conditions (2.2) give, with help of (3.22):

$$\begin{aligned}\left\langle Q_i^2(t)\right\rangle - \langle Q_i(t)\rangle^2 &= \dot{A}_{i0}^2\sigma_q^2(0) + A_{i0}^2\sigma_p^2(0) + 2\dot{A}_{i0}(t)A_{i0}(t)C_{qp}(0) \\ &\quad + \sum_{\ell=1}^{N}\left[\frac{\dot{A}_{i\ell}^2}{\omega_\ell^2} + A_{i\ell}^2\right]E(\omega_\ell, T).\end{aligned} \tag{A.60}$$

The last sum can be rewritten, using expression (A.4) for the $A_{i\ell}$'s, as follows:

$$\begin{aligned}\sum_{\ell=1}^{N}\left[\frac{\dot{A}_{i\ell}^2}{\omega_\ell^2} + A_{i\ell}^2\right]E(\omega_\ell, T) &= \sum_{\ell=1}^{N}\frac{\epsilon_\ell^2}{\omega_\ell^2}\left|\int_0^t \mathrm{d}\tau\; A_{i0}(\tau)e^{\mathrm{i}\omega_\ell\tau}\right|^2 E(\omega_\ell, T) \\ &\quad + \frac{E(\omega_i, T)}{\omega_i^2} + \frac{2\epsilon_i}{\omega_i^2}\int_0^t \mathrm{d}\tau\; A_{i0}(\tau)\cos(\omega_i\tau)E(\omega_i, T).\end{aligned} \tag{A.61}$$

It contains a term explicitly depending on the initial conditions of the central oscillator, and a thermal part. The latter one is made of a term explicitly depending on the initial conditions of the bath oscillator, a sum of the kind $\sum_{\ell=1}\epsilon_\ell^2 \ldots$, which is easily put into integral form by using the strength (3.14), plus an integral containing $A_{i0}(t)$ and an oscillating function of time, multiplied by the coupling ϵ_i of the oscillator. The same structure is obtained for every term of the bath covariance matrix $\sigma^{\rm B}_{ij}$ between any momentum and bath operators.

A.9 Entropy Flow rate terms

Here we determine the explicit form of the entropy flow rate in (7.30) assumed in the thermodynamic limit (7.13) with large cut-off (7.15). By plugging the formal

Heisenberg solution for the left and right bath position operators in the respective energy interaction terms $H_{\rm IL}$ and $H_{\rm IR}$ one gets:

$$\langle H_{\rm IL}(t)\rangle = \left\langle \sum_i Q(t)Q_i(t)\right\rangle = \langle Q(t)\eta_{\rm L}(t)\rangle + \left\langle \int_0^t {\rm d}s\ \dot{K}_{\rm L}(t-s)Q(t)Q(s)\right\rangle. \quad \text{(A.62)}$$

As for the first term of the sum, we use the solution for $Q(t)$ (3.15), the initial absence of system-bath correlation, which implies $\langle Q(0)\eta(t)\rangle = 0$, and the initial absence of correlation between the left and right reservoirs to show that:

$$\begin{aligned}
\langle Q(t)\eta_{\rm L}(t)\rangle &= -\int_0^t {\rm d}t'\ A(t-t')\,\langle \eta_{\rm L}(t')\eta_{\rm L}(t)\rangle \\
&= -\int_0^\infty {\rm d}\omega\ \frac{\gamma_{\rm L}(\omega)}{\omega^2}E(\omega,T_{\rm L})\int_0^t {\rm d}s\ A(s)\cos(\omega s) \quad \text{(A.63)}\\
&= \frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}}D_{qp,T_{\rm L}}. \quad \text{(A.64)}
\end{aligned}$$

According to (A.41), $D_{qp,T_{\rm L}}$ is the anomalous diffusion coefficient associated to the dynamics of the central harmonic oscillator coupled to a single bath at temperature $T_{\rm L}$ in the limit of large cut-off α (A.42), with coupling $\kappa = \kappa_{\rm L}+\kappa_{\rm R}$. In the large cut-off limit the other term in the interaction energy (A.39) can be approximated for $t \gg \alpha^{-1}$ to:

$$\left\langle \int_0^t {\rm d}s\ \dot{K}(t-s)Q(t)Q(s)\right\rangle \simeq -\kappa_{\rm L}\alpha\left\langle Q^2(t)\right\rangle. \quad \text{(A.65)}$$

The time derivative of the averaged left-reservoir interaction term $\left\langle \dot{H}_{\rm IL}(t)\right\rangle$ was reported in (7.32). A similar expression holds for the right reservoir interaction energy.

As for the current (7.29), by using Heisenberg solution $Q_{{\rm L}i}(t)$ in the form (3.9), one gets

$$J_{\rm L}(t) = -\langle P(t)\eta_{\rm L}(t)\rangle - \frac{1}{2}\left\langle \int_0^t {\rm d}s\ \dot{K}_{\rm L}(t-s)\{P(t),Q(s)\}\right\rangle. \quad \text{(A.66)}$$

The first term in the rhs can be written as:

$$\begin{aligned}
\langle P(t)\eta_{\rm L}(t)\rangle &= -\int_0^t {\rm d}t'\ \dot{A}(t-t')\,\langle \eta_{\rm L}(t')\eta_{\rm L}(t)\rangle \\
&= -\int_0^\infty {\rm d}\omega\ \frac{\gamma_{\rm L}(\omega)}{\omega^2}E(\omega,T_{\rm L})\int_0^t {\rm d}s\ \dot{A}(s)\cos(\omega s) \quad \text{(A.67)}\\
&\simeq -\frac{\kappa_{\rm L}}{\kappa_{\rm L}+\kappa_{\rm R}}D_{pp,T_{\rm L}}, \quad \text{(A.68)}
\end{aligned}$$

where according to (A.41), D_{pp,T_L} is the diagonal term of the diffusion matrix associated to the dynamics of the central harmonic oscillator coupled to a single bath at temperature T_L in the large cut-off limit, with coupling $\kappa = \kappa_\mathrm{L}+\kappa_\mathrm{R}$. Just like for the anomalous diffusion coefficient (A.42), one can do the integral in (A.67) and obtain:

$$D_{pp,T_\mathrm{L}}(t) = 2\Gamma \left\langle P^2 \right\rangle_{\mathrm{eq},T_\mathrm{L}} - (\Omega_0^2 A(t) + \dot{A}(t)\frac{d}{dt}) F_{C,T_\mathrm{L}}(t) \tag{A.69}$$

which is expressed through $F_{C,T_\mathrm{L}}(t)$ (A.42) in function of the position equilibrium correlation function $C_\mathrm{L}(t)$ (A.16).

The second term in the rhs of (7.29) is:

$$\begin{aligned}
&\left\langle \int_0^t \mathrm{d}s\ \dot{K}_\mathrm{L}(t-s)\frac{\{P(t),Q(s)\}}{2} \right\rangle = \qquad (A.70)\\
&= \left[-K_\mathrm{L}(t-s)\left\langle \frac{\{P(t),Q(s)\}}{2} \right\rangle \right]\Bigg|_{s=0}^{s=t} + \int_0^t \mathrm{d}s\ K_\mathrm{L}(t-s)\left\langle \frac{\{P(t),P(s)\}}{2} \right\rangle \\
&= -\kappa_\mathrm{L}\alpha \left\langle \frac{\{P(t),Q(t)\}}{2} \right\rangle + K_\mathrm{L}(t)\left\langle \frac{\{P(t),Q(0)\}}{2} \right\rangle + \kappa_\mathrm{L}\left\langle P^2(t) \right\rangle + \mathrm{O}\left(1/\alpha\right) \\
&\simeq -\kappa_\mathrm{L}\alpha \left\langle \frac{\{P(t),Q(t)\}}{2} \right\rangle + \kappa_\mathrm{L}\left\langle P^2(t) \right\rangle,
\end{aligned}$$

where the last equality is valid for $t \gg 1/\alpha$. Then by using the identities (7.29) and (A.70) one gets the analytic expression for $J_\mathrm{L}(t)$ (7.31). Analogously one finds the expression for the right current $J_\mathrm{R}(t)$. Thus in the late-time limit (3.50), after all the transient terms vanish it remains

$$J_\mathrm{L}(\infty) = -J_\mathrm{R}(\infty) = \frac{\kappa_\mathrm{L}\kappa_\mathrm{R}}{\kappa_\mathrm{L}+\kappa_\mathrm{R}}\left[\left\langle P^2 \right\rangle_{\mathrm{eq},T_\mathrm{L}} - \left\langle P^2 \right\rangle_{\mathrm{eq},T_\mathrm{R}} \right]. \tag{A.71}$$

By using explicit expressions for the currents and for the derivative of the interaction energies of the two baths in (7.30) one gets:

$$\begin{aligned}
\dot{S}_\mathrm{e} = \beta_\mathrm{L}&\left[\frac{\kappa_\mathrm{L}}{\kappa_\mathrm{L}+\kappa_\mathrm{R}}(D_{pp,T_\mathrm{L}}(t) + \dot{D}_{qp,T_\mathrm{L}}(t)) - \kappa_\mathrm{L}(\left\langle P^2(t) \right\rangle + \alpha C_{qp}(t)) \right] + \\
\beta_\mathrm{R}&\left[\frac{\kappa_\mathrm{R}}{\kappa_\mathrm{L}+\kappa_\mathrm{R}}(D_{pp,T_\mathrm{R}}(t) + \dot{D}_{qp,T_\mathrm{R}}(t)) - \kappa_\mathrm{R}(\left\langle P^2(t) \right\rangle + \alpha C_{qp}(t)) \right], \qquad (A.72)
\end{aligned}$$

which is correct apart from corrections of $O(1/\alpha)$.

Bibliography

[Agarwal, 1971] Agarwal, G. S. (1971). Brownian motion of a quantum oscillator. *Phys. Rev. A*, 4:739–747.

[Allahverdyan and Nieuwenhuizen, 2000] Allahverdyan, A. E. and Nieuwenhuizen, T. M. (2000). Extraction of work from a single thermal bath in the quantum regime. *Phys. Rev. Lett.*, 85:1799–1802.

[Allahverdyan and Nieuwenhuizen, 2002] Allahverdyan, A. E. and Nieuwenhuizen, T. M. (2002). Testing the violation of the clausius inequality in nanoscale electric circuits. *Phys. Rev. B*, 66:115309.

[Balian, 1999] Balian, R. (1999). Incomplete descriptions and relevant entropies. *American Journal of Physics*, 67(12):1078–1090.

[Balian, 2005] Balian, R. (2005). Information in statistical physics. *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, 36(2):323 – 353.

[Balian and Balazs, 1987] Balian, R. and Balazs, N. (1987). Equiprobability, inference, and entropy in quantum theory. *Annals of Physics*, 179(1):97 – 144.

[Breuer et al., 2009] Breuer, H.-P., Laine, E.-M., and Piilo, J. (2009). Measure for the degree of non-markovian behavior of quantum processes in open systems. *Physical review letters*, 103(21):210401.

[Breuer and Petruccione, 2002] Breuer, H.-P. and Petruccione, F. (2002). *The Theory of Open Quantum Systems*. Oxford University Press, Oxford.

[Breuer and Piilo, 2009] Breuer, H.-P. and Piilo, J. (2009). Stochastic jump processes for non-markovian quantum dynamics. *EPL (Europhysics Letters)*, 85(5):50004.

[Caldeira and Leggett, 1983] Caldeira, A. and Leggett, A. (1983). Path integral approach to quantum Brownian motion. *Physica A: Statistical Mechanics and its Applications*, 121(3):587–616.

[Callen, 1985] Callen, H. (1985). *Thermodynamics and an introduction to thermostatistics*. Wiley.

[Campisi et al., 2009] Campisi, M., Talkner, P., and Hänggi, P. (2009). Fluctuation theorem for arbitrary open quantum systems. *Phys. Rev. Lett.*, 102:210401.

[Cohen and Kottos, 2004] Cohen, D. and Kottos, T. (2004). Quantum dissipation due to the interaction with chaos. *Phys. Rev. E*, 69:055201.

[Colpa, 1978] Colpa, J. H. P. (1978). Diagonalization of the quadratic boson hamiltonian. *Physica A: Statistical Mechanics and its Applications*, 93(3–4):327–353.

[Crooks, 2000] Crooks, G. E. (2000). Path-ensemble averages in systems driven far from equilibrium. *Phys. Rev. E*, 61:2361–2366.

[De Roeck and Maes, 2006] De Roeck, W. and Maes, C. (2006). Steady state fluctuations of the dissipated heat for a quantum stochastic model. *Reviews in Mathematical Physics*, 18(06):619–653.

[Deffner and Lutz, 2011] Deffner, S. and Lutz, E. (2011). Nonequilibrium entropy production for open quantum system. *PRL*, 107:140404.

[Esposito, 2012] Esposito, M. (2012). Stochastic thermodynamics under coarse graining. *Phys. Rev. E*, 85:041125.

[Esposito et al., 2010] Esposito, M., Lindenberg, K., and van den Broeck, C. (2010). Entropy production as correlation between system and reservoir. *New Journal of Physics*, 12(1):013013.

[Esposito and Mukamel, 2006] Esposito, M. and Mukamel, S. (2006). Fluctuation theorems for quantum master equations. *Physical Review E*, 73(4):046129.

[Esposito and Van den Broeck, 2010a] Esposito, M. and Van den Broeck, C. (2010a). Three detailed fluctuation theorems. *Phys. Rev. Lett.*, 104:090601.

[Esposito and Van den Broeck, 2010b] Esposito, M. and Van den Broeck, C. (2010b). Three faces of the second law. I. master equation formulation. *Phys. Rev. E*, 82:011143.

[Fleming et al., 2011] Fleming, C. H., Roura, A., and Hu, B. L. (2011). Exact analytical solutions to the master equation of quantum Brownian motion for a general environment. *Annals of Physics*, 326(5):1207–1258.

[Ford and O'Connell, 2006] Ford, G. W. and O'Connell, R. F. (2006). A quantum violation of the second law? *Phys. Rev. Lett.*, 96:020402.

[Gardiner, 1985] Gardiner, C. (1985). *Handbook of Stochastic Methods: For Physics, Chemistry and Natural Sciences*. Springer series in synergetics, 13. Berlin.

[Gardiner and Zoller, 2004] Gardiner, C. and Zoller, P. (2004). *Quantum Noise:*. Springer Series in Synergetics. Springer.

[Gomez-Marin et al., 2008] Gomez-Marin, A., Parrondo, J. M. R., and Van den Broeck, C. (2008). Lower bounds on dissipation upon coarse graining. *Phys. Rev. E*, 78:011107.

[Grabert et al., 1984] Grabert, H., Weiss, U., and Talkner, P. (1984). Quantum theory of the damped harmonic oscillator. *Zeitschrift für Physik B Condensed Matter*, 55:87–94. 10.1007/BF01307505.

[Haake and Reibold, 1985] Haake, F. and Reibold, R. (1985). Strong damping and low-temperature anomalies for the harmonic oscillator. *Phys. Rev. A*, 32:2462–2475.

[Hänggi and Ludwig Ingold, 2006] Hänggi, P. and Ludwig Ingold, G. (2006). Quantum brownian motion and the third law of thermodynamics. *Acta Physica Polonica B*, 37:1537.

[Hänggi et al., 2008] Hänggi, P., Ludwig Ingold, G., and Talkner, P. (2008). Finite quantum dissipation: the challenge of obtaining specific heat. *New Journal of Physics*, 10(11):115008.

[Hasegawa, 2011] Hasegawa, H. (2011). Classical open systems with nonlinear nonlocal dissipation and state-dependent diffusion: Dynamical responses and the Jarzynski equality. *Physical Review E*, 84(5):051124.

[Hillery et al., 1984] Hillery, M., O'Connell, R. F., Scully, M. O., and Wigner, E. P. (1984). Distribution functions in physics: Fundamentals. *Physics Reports*, 106(3):121–167.

[Hilt and Lutz, 2009] Hilt, S. and Lutz, E. (2009). System-bath entanglement in quantum thermodynamics. *Phys. Rev. A*, 79:010101.

[Hilt et al., 2011] Hilt, S., Shabbir, S., Anders, J., and Lutz, E. (2011). Landauer's principle in the quantum regime. *Phys. Rev. E*, 83:030102.

[Hörhammer and Büttner, 2008] Hörhammer, C. and Büttner, H. (2008). Information and entropy in quantum Brownian motion. *Journal of Statistical Physics*, 133:1161–1174.

[Imparato and Peliti, 2006] Imparato, A. and Peliti, L. (2006). Fluctuation relations for a driven Brownian particle. *Phys. Rev. E*, 74:026106.

[Jarzynski, 1997a] Jarzynski, C. (1997a). Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach. *Phys. Rev. E*, 56:5018–5035.

[Jarzynski, 1997b] Jarzynski, C. (1997b). Nonequilibrium equality for free energy differences. *Phys. Rev. Lett.*, 78:2690–2693.

[Jarzynski, 1999] Jarzynski, C. (1999). Microscopic analysis of Clausius–Duhem processes. *Journal of Statistical Physics*, 96:415–427.

[Jarzynski, 2004] Jarzynski, C. (2004). Nonequilibrium work theorem for a system strongly coupled to a thermal environment. *Journal of Statistical Mechanics: Theory and Experiment*, 2004(09):P09005.

[Jaynes, 1957] Jaynes, E. T. (1957). Information theory and statistical mechanics. *Phys. Rev.*, 106:620–630.

[Kim and Mahler, 2007] Kim, I. and Mahler, G. (2007). The second law of thermodynamics in the quantum Brownian oscillator at an arbitrary temperature. *The European Physical Journal B*, 60:401–408.

[Kim and Mahler, 2010] Kim, I. and Mahler, G. (2010). Clausius inequality beyond the weak-coupling limit: The quantum Brownian oscillator. *Phys. Rev. E*, 81:011101.

[Klimontovich, 1995] Klimontovich, Y. (1995). *Statistical Theory of Open Systems*. Fundamental Theories of Physics Series. Kluwer Acad. Publ.

[Koch et al., 1980] Koch, R. H., Van Harlingen, D. J., and Clarke, J. (1980). Quantum-noise theory for the resistively shunted Josephson junction. *Phys. Rev. Lett.*, 45:2132–2135.

[Kramers, 1940] Kramers, H. A. (1940). Brownian motion in a field of force and the diffusion model of chemical reactions. *Physica*, 7:284.

[Kubo, 1968] Kubo, R. (1968). *Thermodynamics: An advanced course with problems and solutions*. North-Holland Pub. Co.

[Landau and Lifshits, 1958] Landau, L. and Lifshits, E. (1958). *Statistical physics*. Addison-Wesley series in advanced physics. Pergamon Press.

[Lieb, 1976] Lieb, E. H. (1976). The stability of matter. *Rev. Mod. Phys.*, 48:553–569.

[Lindenberg and West, 1990] Lindenberg, K. and West, B. (1990). *The Nonequilibrium Statistical Mechanics of Open and Closed Systems*. Wiley.

[M. Esposito and Mukamel, 2009] M. Esposito, H. H. and Mukamel, D. (2009). Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems. *RMP*, 81:1665.

[Mai and Dhar, 2007] Mai, T. and Dhar, A. (2007). Nonequilibrium work fluctuations for oscillators in non-Markovian baths. *Phys. Rev. E*, 75:061101.

[Nazarov, 2007] Nazarov, Y. V. (2007). Full counting statistics and field theory. *Annalen der Physik*, 16(10-11):720–735.

[Nielsen and Chuang, 2000] Nielsen, M. A. and Chuang, I. (2000). *Quantum computation and quantum information*. Cambridge University Press.

[Nieuwenhuizen and Allahverdyan, 2002] Nieuwenhuizen, T. M. and Allahverdyan, A. E. (2002). Statistical thermodynamics of quantum Brownian motion: Construction of perpetuum mobile of the second kind. *Phys. Rev. E*, 66:036102.

[Ollivier and Zurek, 2001] Ollivier, H. and Zurek, W. H. (2001). Quantum discord: A measure of the quantumness of correlations. *Phys. Rev. Lett.*, 88:017901.

[Peliti, 2011] Peliti, L. (2011). *Statistical Mechanics in a Nutshell*. Princeton University Press.

[Pilgram et al., 2003] Pilgram, S., Jordan, A. N., Sukhorukov, E., and Büttiker, M. (2003). Stochastic path integral formulation of full counting statistics. *Physical review letters*, 90(20):206801.

[Risken, 1989] Risken, H. (1989). *The Fokker–Planck Equation: Methods of Solutions and Applications*. Springer, 2nd edition.

[Ruelle, 1969] Ruelle, D. (1969). *Statistical mechanics: Rigorous results*. Mathematical physics monograph series. W. A. Benjamin.

[Saito and Dhar, 2007] Saito, K. and Dhar, A. (2007). Fluctuation theorem in quantum heat conduction. *Physical Review Letters*, 99(18):180601.

[Seifert, 2005] Seifert, U. (2005). Entropy production along a stochastic trajectory and an integral fluctuation theorem. *Phys. Rev. Lett.*, 95:040602.

[Seifert, 2008] Seifert, U. (2008). Stochastic thermodynamics: Principles and perspectives. *The European Physical Journal B*, 64:423–431.

[Simon et al., 1994] Simon, R., Mukunda, N., and Dutta, B. (1994). Quantum-noise matrix for multimode systems: U(n) invariance, squeezing, and normal forms. *Phys. Rev. A*, 49:1567–1583.

[Speck and Seifert, 2007] Speck, T. and Seifert, U. (2007). The Jarzynski relation, fluctuation theorems, and stochastic thermodynamics for non-markovian processes. *Journal of Statistical Mechanics: Theory and Experiment*, 2007(09):L09002.

[Spohn and Lebowitz, 2007] Spohn, H. and Lebowitz, J. L. (2007). *Irreversible Thermodynamics for Quantum Systems Weakly Coupled to Thermal Reservoirs*, pages 109–142. John Wiley & Sons, Inc.

[Suominen et al., 1992] Suominen, K.-A., Garraway, B. M., and Stenholm, S. (1992). Wave-packet model for excitation by ultrashort pulses. *Phys. Rev. A*, 45:3060–3070.

[Talkner et al., 2007] Talkner, P., Lutz, E., and Hanggi, P. (2007). Fluctuation theorems: Work is not an observable. *arXiv preprint cond-mat/0703189*.

[Thirring, 1981] Thirring, W. (1981). *Quantum mechanics of atoms and molecules*. A Course in Mathematical Physics. Springer-Verlag.

[Ullersma, 1966] Ullersma, P. (1966). An exactly solvable model for Brownian motion: I. Derivation of the Langevin equation. *Physica*, 32(1):27–55.

[Vidal and Werner, 2002] Vidal, G. and Werner, R. F. (2002). Computable measure of entanglement. *Phys. Rev. A*, 65:032314.

[Williamson, 1936] Williamson, J. (1936). On the algebraic problem concerning the normal forms of linear dynamical systems. *Amer. J. Math.*, 58(1):141–163.

[Yukawa, 2001] Yukawa, S. (2001). The second law of steady state thermodynamcs for nonequilibrium quantum dynamics. *arXiv:cond-mat/0108421*.

[Zamponi et al., 2005] Zamponi, F., Bonetto, F., Cugliandolo, L. F., and Kurchan, J. (2005). A fluctuation theorem for non-equilibrium relaxational systems driven by external forces. *Journal of Statistical Mechanics: Theory and Experiment*, 2005(09):P09013.

[Zurek, 2003] Zurek, W. H. (2003). Decoherence, einselection, and the quantum origins of the classical. *Rev. Mod. Phys.*, 75:715–775.

[Zwanzig, 2001] Zwanzig, R. (2001). *Nonequilibrium Statistical Mechanics*. Oxford University Press, USA.